IN THE UNITED STATES PATENT AND TRADEMARK OFFICE
(Docket No. 05-720-US1)

In the Application of: Kouvetakis, et al.)	
)	
)	Examiner: RAO,
)	SHRINIVAS H.
Serial No.: 10/559,979)	
)	Group Art Unit: 2814
Filing Date: December 8, 2005)	
)	Confirmation No.: 6573
For: $Si_xSn_yGe_{1-x-y}$ and Related Alloy)	
Heterostructures Based on Si, Ge, and Sn)	
)	

APPELLANTS' BRIEF IN SUPPORT OF THE
APPEAL TO THE BOARD OF PATENT APPEALS AND INTERFERENCES

Dear Sir:

This Appeal Brief is submitted pursuant 37 C.F.R. § 41.37, within five months from the July 6, 2007 mailing of the Notice of Appeal as accompanied by a Petition for Extension of Time under 37 CFR 1.136(a) of three months.

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I. Real Party in Interest

The real party in interest is the Arizona Board of Regents, Acting for and on Behalf of Arizona State University, A Corporate Body Organized under Arizona Law.

II. Related Appeals and Interferences

Applicant is not aware of any related appeals or interferences.

III. Status of Claims

Claims 1 – 27 are presently pending in the application. Claims 1 – 12, 14 – 17, and 19 – 27 stand rejected for allegedly being anticipated by Soref *et al.*, U.S. 5,548,128 ("Soref"). Claims 3, 13, and 18 stand rejected for allegedly being anticipated by Fieselmann, U.S. 4,777,023 ("Fieselmann"). Claims 9 – 17 stand rejected as allegedly being indefinite under 35 USC §112, 2nd paragraph. The rejection of claims 1 – 27 are presently appealed.

IV. Status of Amendments

Claims 1 – 27 stand as amended in Applicant's "Response to the Office Action Mailed June 16, 2006."

V. Summary of Claimed Subject Matter

Independent claim 1 recites a semiconductor structure comprising a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer. (Paragraph [0011], line 2 and exemplified in Figure 3) The essentially single phase nature of the $Ge_{1-x-y}Si_xSn_y$ layer is described at paragraphs [0012], [0015], [0037] and Figure 2. Such substrates include silicon (Claims 2 and 6; Paragraph [0011]). In the formula Sn_zGe_{1-z}, z can be about 0.01 to about 0.05 (Claims 4 and 6; Paragraphs [0011], [0012], [0032] – [0034], and Table 1) . In the formula $Ge_{1-x-y}Si_xSn_y$, x can be about 0.01 to about 0.25; and y can be about 0.01 to about 0.11 (Claims 5 and 6; Paragraphs [0011], [0012], [0032] – [0034], and Table 1). The $Ge_{1-x-y}Si_xSn_y$ layer itself can be strained (Claim 7; Paragraphs [0011], [0012],

[0017], [0032], and Figure 4) or relaxed (Claim 8; Paragraphs [0011], [0012], [0018] [0032], and Figure 5). Further, the Sn_zGe_{1-z} and $Ge_{1-x-y}Si_xSn_y$ layers can be lattice-matched (Claim 25; Paragraphs [0017], [0038], and Figure 4).

Dependent claim 9 describes a method to prepare the semiconductor structure according to claim 1, comprising the steps of, providing a substrate, depositing a Sn_zGe_{1-z} layer over the substrate; and depositing a $Ge_{1-x-y}Si_xSn_y$ layer over the Sn_zGe_{1-z} layer (Paragraph [0032]). The $Ge_{1-x-y}Si_xSn_y$ layer can be deposited by precursor chemical vapor deposition, wherein the precursor chemical vapor comprises SnD_4 and H_3SiGeH_3 (Claim 10; Paragraphs [0010], [0022], [0033]). The Sn_zGe_{1-z} layer can be deposited by precursor chemical vapor deposition, wherein the precursor chemical vapor comprises SnD_4 and Ge_2H_6 (Claim 11; Paragraphs [0022] and [0033]). In the claimed method, the substrate may comprise silicon (Claims 12 and 16; paragraph [0032]). The method can further include annealing the Sn_zGe_{1-z} layer prior to depositing the $Ge_{1-x-y}Si_xSn_y$ layer (Claim 13; Paragraph [0036]). The method can be used to prepare Sn_zGe_{1-z} layers where z is about 0.01 to about 0.05 (Claims 14 and 16; Paragraphs [0011], [0012], [0032] – [0034], and Table 1) and $Ge_{1-x-y}Si_xSn_y$ layers wherein x is about 0.01 to about 0.25; and y is about 0.01 to about 0.11 (Claims 15 and 16; Paragraphs [0011], [0012], [0032] – [0034], and Table 1). The precursor chemical vapor to form the $Ge_{1-x-y}Si_xSn_y$ layer can be performed at a temperature of about 310°C to about 375°C (Claim 17; Paragraph [0033] - [0034]).

Independent claim 3 recites a method for synthesizing a compound having the molecular formula $H_3Si-GeH_3$, the method comprising combining $H_3SiO_3SCF_3$ with $KGeH_3$ under conditions whereby $H_3Si-GeH_3$ is obtained (Paragraph [0029]). The combining can take place at about -60°C (Claim 18; Paragraphs [0029] - [0030]).

Independent claim 19 recites an alloy of the formula, $Ge_{1-x-y}Si_xSn_y$, wherein x is about 0.01 to about 0.25 and y is about 0.01 to about 0.11 (Paragraphs [0033] – [0034] and Table 1). In the claimed alloy, x can be about 0.13 to about 0.20 (Claim 20; Paragraphs [0033] – [0034] and Table 1). In other alloys, y can be about 0.07 to about 0.11 (Claim 21; Paragraph [0034] and Table 1) or about 0.01 to about 0.06 (Claim 22; Paragraphs [0034] and Table 1).

Such alloys can be used in either (i) a semiconductor structure comprising a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and a layer of the alloy of Claim 19 formed over the

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Sn_zGe_{1-z} layer (Claim 23; Paragraphs [0011], [0014] – [0018], [0034], and Table 1); or a structure comprising: a Sn_zGe_{1-z} layer and a layer of the alloy of Claim 19 formed over the Sn_zGe_{1-z} layer (Claim 27; Paragraphs [0012] and [0032] – [0036]). In the semiconductor structures, the substrate can comprise silicon (Claim 24; Paragraph [0011]) and the Sn_zGe_{1-z} and $Ge_{1-x-y}Si_xSn_y$ layers can be lattice-matched (Claim 26; Paragraphs [0017], [0038], and Figure 4).

VI. *Grounds of Rejection to be Reviewed on Appeal*

1. Whether Claims 1 – 12, 14 – 17, and 19 – 27 are unpatentable under 35 U.S.C §102(b) over U.S. 5,548,128 ("Soref").

2. Whether Claims 3, 13, and 18 are unpatentable under 35 U.S.C §102(b) over U.S. 4,777,023 ("Fieselmann").

3. Whether Claims 9 – 17 are unpatentable under 35 U.S.C §112, 2nd paragraph.

VII. *Argument*

A. Rejection of Claims 1 – 12, 14 – 17, and 19 – 27 under 35 USC §102(b)

Claims 1 – 12, 14 – 17, and 19 – 27 stand rejected for allegedly being anticipated by Soref *et al.*, U.S. 5,548,128 ("Soref"). The Applicants respectfully traverse.

1. Independent Claim 1

a. Soref does not expressly or inherently describe all the present claim limitations.

Independent claim 1 presently stands rejected for allegedly being anticipated by Soref, however, Applicant submits that Soref does not anticipate, either expressly or inherently, at least the following limitations of claim 1:

(i)   An essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer.

(ii)   The combination of (a) a substrate, (b) a Sn_zGe_{1-z} layer, and (c) an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer, where the Sn_zGe_{1-z} layer is formed

over the substrate, and the essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer.

For a claim to be anticipated by the prior art, under 35 USC §102, the reference must recite all limitations of the allegedly anticipated claim. "A claim is anticipated only if each and every element as set forth in the claim is found, either expressly or inherently described, in a single prior art reference." *Verdegaal Bros. v. Union Oil Co. of California*, 814 F.2d 628, 631, 2 USPQ2d 1051, 1053 (Fed. Cir. 1987) MPEP 2131. The fact that a certain result or characteristic <u>may</u> occur or be present in the prior art is not sufficient to establish the inherency of that result or characteristic. *In re Rijckaert*, 9 F.3d 1531, 1534, 28 USPQ2d 1955, 1957 (Fed. Cir. 1993) (emphasis in original). "To establish inherency, the extrinsic evidence 'must make clear that the missing descriptive matter is necessarily present in the thing described in the reference, and that it would be so recognized by persons of ordinary skill. Inherency, however, may not be established by probabilities or possibilities. The mere fact that a certain thing may result from a given set of circumstances is not sufficient.' " *In re Robertson*, 169 F.3d 743, 745, 49 USPQ2d 1949, 1950-51 (Fed. Cir. 1999), MPEP 2112 (IV).

Presently, claim 1 reads as follows (emphasis added):

> 1. A semiconductor structure comprising: ***a substrate***, ***a Sn_zGe_{1-z} layer*** formed over the substrate, and ***an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer*** formed over the Sn_zGe_{1-z} layer.

(i)   Soref does not disclose an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer

Upon review of Soref, Applicants note the following discussions regarding "SiGeSn layers" therein:

<u>A. the Abstract (emphasis added):</u>

> *Silicon-based laser diodes, optical amplifiers, electrooptical modulators, and photodetectors in which the active region consists of a pseudomorphic GeSn multiple quantum well stack. Each quantum well is tensile-strained $Ge_{1-x}Sn_x$ layer sandwiched between compressively strained barriers of $Ge_{1-y}Sn_y$, with x-0.1, x<y and y=0.15. The GeSn quantum wells have a strain-induced direct gap for strongly allowed band-to-band transitions in the infrared range. **The quantum well stack is grown upon a relaxed SiGeSn alloy buffer portion whose composition is graded up from a lattice match at the silicon substrate interface to a Ge or GeSn composition at buffer's top surface.** Doped cladding layers are*

added, so that the devices have a p-i-n diode structure. The monolithic integrated Column IV devices have a rib waveguide structure, where desired, and operate typically in the 2 to 3 micron wavelength range.

Herein, Soref notes that the "SiGeSn alloy buffer portion" is graded from Si to either Ge or GeSn, however, this statement does not describe any material which necessarily contains Si, Ge, and Sn in an essentially single phase form, as presently claimed. Further discussion of the nature of the "SiGeSn alloy buffer portion" is presented by Soref as follow.

B. at Column 3, lines 25 – 29 (emphasis added),

> *The strain-relieved buffer under the stack can be constructed from a spatially **varying (graded)** composition alloy of SiGeSn. At the **Si wafer, the buffer layer 21 is Si-like**. At the **top surface of the buffer layer 19, the alloy is like GeSn**, for example, $Ge_{0.92}Sn_{0.08}$.*

While Soref notes that the buffer layers "can be constructed from a spatially varying (graded) composition alloy of SiGeSn" (see, Col. 3, ll. 25 – 27), a definition for a "varying (graded) composition alloy of SiGeSn" follows at Col. 3, lines 27 – 29, *"At the Si wafer, the buffer layer 21 is Si-like. At the top surface of the buffer layer 19, the alloy is like GeSn, for example, $Ge_{0.92}Sn_{0.08}$."*

Applicants submit that Soref is merely using the term "SiGeSn layer" to refer to the graded compositions which satisfy the stated compositions at the faces of layers #19 and #21. Neither discussion of the *"composition alloy SiGeSn"* of describes an essentially single phase SiGeSn material as presently claimed.

C. at Column 3, lines 33 – 44 (emphasis added),

> *The upper buffer layer 11 can be p-doped, and the remaining intermediate layers of the stack are substantially undoped. However, the device can also be p-i-p or n-i-n if desired. **It may be difficult technically to grade the composition of the SiGeSn lower buffer from pure silicon up to germanium-tin**. In that case, two buffer layers can be grown upon the silicon substrate: for example, lower buffer layer 21 could be relaxed SiGe, **with a composition that varied** between pure Si and pure Ge; and lower buffer 19 would be a relaxed alloy of GeSn, whose **composition varied** from pure Ge to $Ge_{0.95}Sn_{0.05}$. Both lower buffers could be doped n-type.*

Further, Soref acknowledges, *"It may be difficult technically to grade the composition of the SiGeSn lower buffer from pure silicon up to germanium-tin"* (see, Col. 3, ll. 36 – 38). As an

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alternative, Soref suggests the use of two separate layers (i.e., layers #19 and #21), which themselves are also **graded compositions**, "*In that case, two buffer layers can be grown upon the silicon substrate: for example, lower buffer layer 21 could be relaxed SiGe, with a composition that varied between pure Si and pure Ge; and lower buffer 19 would be a relaxed alloy of GeSn, whos composition varied from pure Ge to $Ge_{0.95}Sn_{0.05}$*" (see, Col. 3, ll. 38 – 44).

Therefore, in combination with the preceding quotation (B), for the buffer layer (#19) between the substrate (#1) and the active GeSn layer (#13') Soref describes the use of either,

(i) a single graded layer containing Si, Ge, and Sn, whose composition is "Si-like" at the Si substrate and "GeSn-like" at the active layer (#13'); or

(ii) or two separate buffer layers, one graded from pure Si to pure Ge (#21) and the second graded from pure Ge to $Ge_{0.95}Sn_{0.05}$ (#19).

Neither alternative describes the presently claimed essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer.

D. Claim 16 therein (emphasis added):

16. A semiconductor optical device comprising:
(a) an active region made up of a multiple quantum well stack having in-plane tensile strained germanium-tin alloy quantum wells and germanium-tin alloy barriers, said quantum well stack having given lattice constants, and wherein the quantum wells have an atomic percentage of tin of 5% to 15%, enabling a direct bandgap to exist between the n=1 conduction subband and the n=1 valence subband of the multiple quantum wells of said stack and wherein said barriers have an atomic percentage of tin of 3% to 6% more than the percentage of tin in the quantum wells and are compressively strained in-plane for producing symmetric strain for the quantum well stack to enable a thick high quality stack to be formed;
*(b) a doped relaxed **SiGeSn graded composition** lower buffer portion positioned below the stack, grown upon and contacting a substrate selected from the group consisting of Si and Ge;*
(c) a doped relaxed GeSn composition upper buffer portion positioned above the stack, and wherein said upper and lower buffer layers each have a zincblend lattice constant that is halfway between the lattice constant of the wells and the lattice constant of the barriers; and
(d) a first electrode coupled to said upper buffer layer portion and a second electrode coupled to said lower buffer layer portion.

Claim 16 merely echoes the description of the specification and abstract, particularly in noting that the claimed semiconductor optical device of Soref contains "a doped relaxed SiGeSn graded composition lower buffer portion." Again, such a description does not teach an essentially single phase SiGeSn material as presently claimed.

Applicants note that in each of the preceding quotations from Soref, (A) – (D), the document consistently teaches the use of graded compositions comprising Si, Ge, and Sn. At no point does Soref teach the use of an essentially single phase material for the SiGeSn layer. Further, at no point does Soref teach that all three constituent elements of the SiGeSn layer form a single alloy; rather, Soref only teaches that the layer has particular boundary conditions for the "SiGeSn layers" used in the described devices. Namely, those boundary conditions require that the SiGeSn layer be "Si-like" at the substrate surface and "GeSn-like" at the opposite surface (*i.e.,* at Col. 3, lines 27 – 29). Neither boundary condition describes the essentially single phase SiGeSn layer as presently claimed.

The Office has further alleged on page 6 through 7 of the Final office action (emphasis original),

> *The layer [SiGeSn layer] <u>can be constructed</u>...i.e. the strained layer can be spatially varying or not spatially varying and in the embodiment wherein the strained is not spatially varying applicants' arguments are not persuasive.*
>
> *It is noted that it is readily apparent to one skilled in the art that Soren's [sic] uses the same material for the same material (Si-Ge-Sn) alloy for the same purpose (strain free layers) therefore what is true for Applicant's (Si-Ge-Sn alloys are particularly suitable to form highly uniform (i.e. substantiall single phase) is also true for Soren [sic]. Further Applicants' specification para 0032 states (in relevant parts) "materials like Si-ge-Sn alloys are chosen because they form highly uniform layers , all of which make it clear to one of ordinary skill in the art , that Soren [sic] also discloses its layer to be highly uniform i.e. consists elemental uniformity of material that is consistent with single phase alloy layer.*

The Office has raised two issues here; one appears to invoke an alleged inherent disclosure of the presently claimed *essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer*; and the second is an alleged admission by Applicants regarding the nature of SiGeSn alloys. On each point, Appicants respectfully submit that the Office is incorrect.

First, Applicants submit that the Office has not met its burden of proof to establish that the missing descriptive matter (*i.e.,* a non-graded "SiGeSn" layer) is necessarily present in Soref

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to support a rejection based on inherency. As stated in *Ex Parte Levy, 17 USPQ2d, 1461, 1464 (citing In re King, 801 F.2d 1324), "In relying upon the theory of inherency, the examiner must provide a basis in fact and/or technical reasoning to reasonable support the determination that the alledgedly inherent characteristic necessarily flows from the prior art."*

In *Ex Parte Levy,* claims to a biaxially oriented polymeric balloon (*e.g.,* a catheter balloon) were originally rejected by the Office over a reference (Schjeldahl) which allegedly inherently disclosed a balloon having the same properties (i.e., biaxially oriented). The Schjeldahl reference characterized a starting material for the balloon as biaxially oriented, while the nature of a balloon formed by blow molding of the starting material was not defined. The Office based its rejection on a belief that, "*since the reference produces a biaxially oriented article, clearly a stretching step must be used... Since Schjeldahl et al produces a biaxially oriented article it follows that a stretching step must be used in the injection blow molding process.*" However, the BPAI found that (*ibid*, at 1463), "*The inescapable facts are that Schjeldahl does not disclose a biaxially oriented catheter balloon and does not mention a stretching step.*"

Analagous to *Ex Parte Levy,* Soref does not mention a single-phase SiGeSn layer, only graded compositions (supra). Further, Soref does not provide any working examples, or any other discussion for that matter, revealing the process conditions employed to produce any "SiGeSn" layer, much less the single-phase SiGeSn layer as presently claimed. The Office has not offered any evidence to provide a basis in fact and/or technical reasoning that a single-phase SiGeSn layer necessarily flows from the teachings of Soref.

On the second point, Applicants submit that paragraph [0032] of the instant specification has nothing to do with the SiSnGe layer or alloy as asserted and relied upon by the Office. The referenced paragraph of the specification reads, in whole, (emphasis added),

> *We initially investigated the growth of $Si_{1-x-y}Ge_xSn_y$ directly on Si(100) using $Ge_{1-x}Sn_x$ (x=2-4 at. %) buffer layers. We chose **$Ge_{1-x}Sn_x$ alloys** as buffer layers because they possess crystallographic, morphological and mechanical properties that make them uniquely suitable for use as templates on Si substrates. **These materials** grow as highly uniform, strain-free layers with smooth and continuous surface morphologies (typical AFM rms values are 0.5 and 1.4 nm) and display extremely low concentrations of threading defects, particularly those that extend to the uppermost surface (the quality of pure Ge films grown on Si by*

*similar methods is much worse). In addition, **they** are high compressibility (softer) solids compared to either Si and $Si_{1-x-y}Ge_xSn_y$ and thereby **can act as potential spacers** that can conform structurally and readily absorb the differential strain imposed by the more rigid Si and Si-Ge-Sn.*
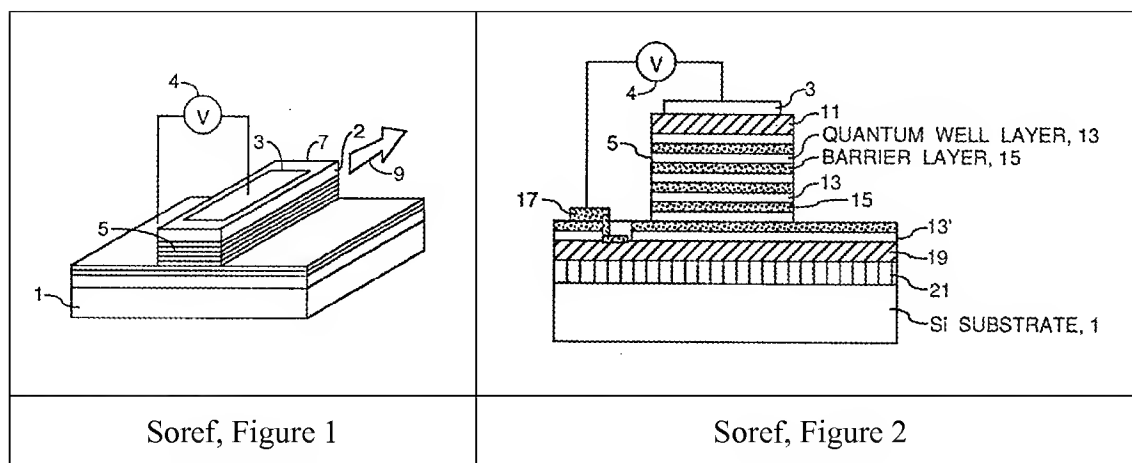
Rather paragraph [0032] is wholly concerned with the **$Ge_{1-x}Sn_x$ buffer layer** (note the comparisons to the SiGeSn layer in the final sentence). In fact, Applicants have been unable to find any statement in the instant specification which contains, *"materials like Si-Ge-Sn alloys are chosen because they form highly uniform layer..."* as quoted by the Office in the present action. Thus, Applicants have not admitted, and do not admit, that *"Si-Ge-Sn alloys are chosen because they form highly uniform layer,"* in fact, such a statement would have been impossible by Applicants as the Si-Ge-Sn alloys were experimentally unknown prior to the instant invention (see, Specification, paragraphs [0007] and [0010}.

(ii)   Soref does not disclose the combination of (a) a substrate, (b) a Sn_zGe_{1-z} layer, and (c) an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer, where the Sn_zGe_{1-z} layer is formed over the substrate, and the essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer.

Additionally, for Soref to anticipate instant claim 1, it must also disclose the recited combination of the constituent elements; that is, a Sn_zGe_{1-z} layer formed over a substrate, and an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer. In the present rejection, the Office alleges that Soref teaches, according to the numbering in Figures 1 and 2 of Soref,

> *"a substrate (Soref figs. 1 or 2 #1), a Sn_zGe_{1-z} layer formed over the substrate (Soref figs 1 or 2 #13 col. 2 line 45-47), and an essentially single-phase $Ge_{1-x-y}Sn_xSi_y$ layer formed over the Sn_zGe_{1-z} layer (Soref figs. 1 or 2 #19, col. 3 line 44-45)."*

Again, for convenience, Figures 1 and 2 of Soref read as follow:
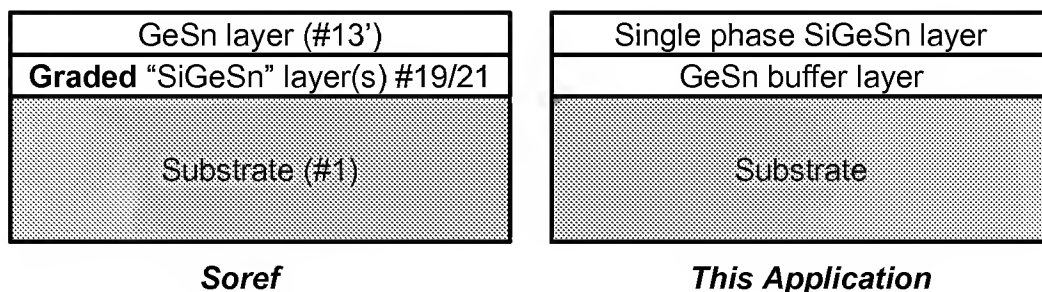
| Soref, Figure 1 | Soref, Figure 2 |

where individual components are (see Column 2, Lines 41 – 58): **3** – ohmic contact **4** – current source; **5** – reflective end facet; **11** – relaxed upper buffer layer (p- or n-doped, see Col. 4, Lines 19 – 23); **13** – GeSn quantum wells (QW); **13'**- 'active QW layer'; **15** – barrier layers; **17** – ohmic contact; **19** – n-doped buffer layer; and **21** - n-doped buffer layer.

Applicants note that according to Figure 2, layer #19 (a spatially graded buffer layer of "SiGeSn"; see, Col. 3, lines 25 - 29) is formed over the substrate *(layer #1)*, and layer #13 (a GeSn quantum well; see, Col. 2, lines 45 – 46) is formed over layer #19. The only layer shown between the "SiGeSn layer" (#19) and the substrate (#1) is layer #21, not layer #13 as alleged by the Office.

Layer #21 is the "lower buffer layer" which is described as *"relaxed SiGe with a composition that varied between pure Si and pure Ge"* (see Col. 3, ll. 33 – 44, *supra*). Accordingly, Soref teaches a *graded* "SiGeSn layer" (layer #19) formed over the substrate (layer #1) with a GeSn layer (layer #13) formed over the "SiGeSn" layer.

The differences between Soref can be readily seen in the following figure, in Soref, the GeSn layer is formed on top of the "SiGeSn" layer while in the instant application and claims, the GeSn layer is formed on the substrate and provides for the formation of the SiGeSn thereover.

GeSn layer (#13')	Single phase SiGeSn layer
Graded "SiGeSn" layer(s) #19/21	GeSn buffer layer
Substrate (#1)	Substrate

Soref	*This Application*

The combination of layers disclosed in Soref is different than the instantly claimed arrangement. Further, as layers #19 and #21 are buffer layers, Sooref does not discuss or suggest to reverse the order of layers #13' and #19 or #21; therefore, Sref does not inherenty teach the presently claimed structure.

To establish a *prima facie* case for anticipate Claim 1 by Soref, Soref must expressly or inherently disclose the claimed composition and combination of layers. Based on all of the above, Applicants submit that Soref describe neither the instantly claimed essentially single-phase SiGeSn layer nor the proper order of layers in the presently claimed structures, and therefore, the Office has failed to establish a *prima facie* case for anticipation of instant Claim 1.

b. Soref is not enabling prior art

Applicants maintain that the "essentially single phase" SiGeSn layer of Claim 1 is neither explicitly or inherently anticipated by Soref, nor is the presently claimed structure described. However, even *if* the Office maintains that the "essentially single phase" SiGeSn layer **and** the combination of layers in the presently claimed structures are disclosed, Applicants submit that Soref is not enabling for such compositions comprising an essentially single phase SiGeSn layer.

"In determining that quantum of prior art disclosure which is necessary to declare an applicant's invention 'not novel' or 'anticipated' within section 102, the stated test is whether a reference contains an 'enabling disclosure'... ." *In re Hoeksema,* 399 F.2d 269, 158 USPQ 596 (CCPA 1968). The disclosure in an assertedly anticipating reference must provide an enabling disclosure of the desired subject matter; mere naming or description of the subject matter is insufficient, if it cannot be produced without undue experimentation. *Elan Pharm., Inc. v. Mayo Found. For Med. Educ. & Research,* 346 F.3d 1051, 1054, 68 USPQ2d 1373, 1376 (Fed. Cir.

2003). **MPEP 2121.01.** Where a process for making the compound is not developed until after the date of invention, the mere naming of a compound in a reference, without more, cannot constitute a description of the compound. *In re Hoeksema*, 399 F.2d 269, 158 USPQ 596 (CCPA 1968). **MPEP 2121.02(I). (Emphasis added)**

As stated in the present specification, at the time of filing, the presently claimed SiGeSn compositions were experimentally unknown and their properties only had been investigated by theoretical means (see, Specification, paragraph [0007]). The instant application describes for the first time, a method for preparing such a SiGeSn compositions (see, Specification, [0010]).

The synthetic methods mentioned in Soref are chemical vapor deposition (CVD) and molecular beam epitaxy (MBE) (see, Col. 2, lines 11 – 19). Upon or review, it does not appear that Soref contains any further discussion of the preparation of any of the layers. Applicants note that the discussion at Col. 2, lines 11 – 19 is related to **GeSn** layers and not any "SiGeSn" layer:

> *The active material here is a **germanium-tin** alloy. Experiments have been reported in the literature where several percent of alpha-tin (as much as 25%) were incorporated in a germanium lattice by means of "epitaxial stabilization" which is a form of non-equilibrium growth. The growth techniques are chemical vapor deposition (CVD) and molecular beam epitaxy (MBE). The growth procedures are similar to those used for $Si_{1-x}Ge_x$ upon Si, thus the **GeSn growth** is expected to be quite feasible.*

Soref is silent with respect to any methods for preparing any "SiGeSn layer", regardless of whether it is graded or a single phase.

Therefore, at the time of filing the instant application, one skilled in the art, given the Soref reference, would require undue experimentation to prepare the claimed essentially single-phase SiGeSn layers, as evidenced by the substantial lack of known methods for preparing the same in the art. Without a proper description of how to make the claimed essentially single phase SiGeSn layer, and without the knowledge available in the art, one skilled in the art would not be able to make the claimed essentially single phase SiGeSn layer based solely on the Soref reference. For example, MPEP 2121.02, "Compounds and compositions – What Constitutes Enabling Prior Art", states in relevant portions,

> *I.< ONE OF ORDINARY SKILL IN THE ART MUST BE ABLE TO MAKE OR SYNTHESIZE*
> *Where a process for making the compound is not developed until after the date of invention, the mere naming of a compound in a reference, without more, cannot constitute a description of the compound. In re Hoeksema, 399 F.2d 269, 158 USPQ 596*

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(CCPA 1968). Note, however, that a reference is presumed operable until applicant provides facts rebutting the presumption of *>operability<. In re Sasse, 629 F.2d 675, 207 USPQ 107 (CCPA 1980). Therefore, applicant must provide evidence showing that a process for making was not known at the time of the invention. See the following paragraph for the evidentiary standard to be applied.

II.< A REFERENCE DOES NOT CONTAIN AN "ENABLING DISCLOSURE" IF ATTEMPTS AT MAKING THE COMPOUND OR COMPOSITION WERE UNSUCCESSFUL BEFORE THE DATE OF INVENTION

When a prior art reference merely discloses the structure of the claimed compound, evidence showing that attempts to prepare that compound were unsuccessful before the date of invention will be adequate to show inoperability. In re Wiggins, 488 F.2d 538, 179 USPQ 421 (CCPA 1971).

In support of Applicants assertion that the presently claimed materials were experimentally unknown at the time of filing of the instant application, Applicants refer to Aella, *et al. Appl. Phys. Lett.* **2004**, *84*, 888 ('Aella'), which states in the first paragraph in the left-hand column of page 888, *"Our own preliminary study describes the first successful growth of this material [Si-Ge-Sn]*," referencing Bauer *et al., Appl. Phys. Lett.* **2003**, *83*, 2163 ('Bauer'). Both Aella[1] and Bauer[2] were introduced as evidence in the instant application in the Information Disclosure Statement, filed by Applicant on December 8, 2006. Each was considered and entered into the record by the examiner by their consideration and initialing of the IDS on March 2, 2007. Copies of both Aella and Bauer are included in Section IX of this Appeal Brief. Both peer-reviewed references illustrate that it was accepted in the art, at the time of filing of the instant application[3], that methods for making the instantly claimed materials were unknown until the instant invention thereof. Aella published on February 9, 2004 and Bauer published on September 15, 2003.

c. Conclusion

For each of the preceding reasons, that Soref does not explicitly or inherently disclose an essentially single phase SiGeSn layer as presently claimed nor explicitly or inherently disclose

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[1] See Document No. 75

[2] See Document No. 70

[3] June 13, 2003: The instant application entered the U.S. National Phase under 35 USC §371 on December 8, 2005, from PCT/US2004/018969, filed June 14, 2004, which claims the priority, under 35 USC §363 and §119(e), of the filing date of U.S. Provisional Application Serial No. 60/487,480, filed on June 13, 2003.

the claimed combination of layers; and that Soref is not enabled for any method for preparing the instantly claimed essentially single phase SiGeSn layers, Applicants submit that Soref does not anticipate Claim 1. Applicants respectfully request reconsideration and withdrawal of the rejection.

2. Independent Claim 9

In the present Final Office Action, Claim 9 stands rejected for allegedly being anticipated by Soref. Claim 9 presently reads, (emphasis added)

> *9. A method to prepare the semiconductor structure according to claim 1, comprising the steps of,*
>
> > *providing a substrate;*
> >
> > *depositing a Sn_zGe_{1-z} layer over the substrate; and*
> >
> > *depositing a $Ge_{1-x-y}Si_xSn_y$ layer over the Sn_zGe_{1-z} layer.*

To anticipate instant Claim 9, Soref must describe a method for *"depositing a $Ge_{1-x-y}Si_xSn_y$ layer over the Sn_zGe_{1-z} layer"* where the $Ge_{1-x-y}Si_xSn_y$ layer is an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer (*i.e.,* the structure according to claim 1). Applicants submit that Soref does not describe (i) an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer as presently claimed, (ii) a semiconductor structure as prepared by the presently claimed method, (iii) or any methods which are capable of producing an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer.

As previously noted with respect to the outstanding rejection of Claim 1, upon review of Soref, Applicants note that "SiGeSn layers" are discussed in Soref in the Abstract, at Column 3, lines 25 – 29, at Column 3, lines 33 – 44, and Claim 16 (*supra*). Applicants note that Soref describes buffer layers (layers #19 and 21, Figure 2) between a substrate (#1) and "active quantum wells" containing GeSn (#13') as a "SiGeSn layer" (see, Figure 2 and Col. 2, ll. 52 – 55). The buffer layers "can be constructed from a spatially varying (graded) composition alloy of SiGeSn" (see, Col. 3, ll. 25 – 27). A definition for a "varying (graded) composition alloy of SiGeSn" follows at Col. 3, lines 27 – 29, *"At the Si wafer, the buffer layer 21 is Si-like. At the top surface of the buffer layer 19, the alloy is like GeSn, for example, $Ge_{0.92}Sn_{0.08}$."*

Soref is merely using the term "SiGeSn layer" to refer to graded compositions which satisfy the stated compositions at the faces of layers #19 and #21.

Further, Soref acknowledges, *"It may be difficult technically to grade the composition of the SiGeSn lower buffer from pure silicon up to germanium-tin"* (see, Col. 3, ll. 36 – 38). As an alternative, Soref suggests the use of two separate layers (i.e,, layers #19 and #21), which themselves are also graded compositions, *"In that case, two buffer layers can be grown upon the silicon substrate: for example, lower buffer layer 21 could be relaxed SiGe, with a composition that varied between pure Si and pure Ge; and lower buffer 19 would be a relaxed alloy of GeSn, whos composition varied from pure Ge to $Ge_{0.95}Sn_{0.05}$"* (see, Col. 3, ll. 38 – 44).

Therefore, for the buffer layer (#19) between the substrate (#1) and the active GeSn layer (#13)' Soref describes the use of either
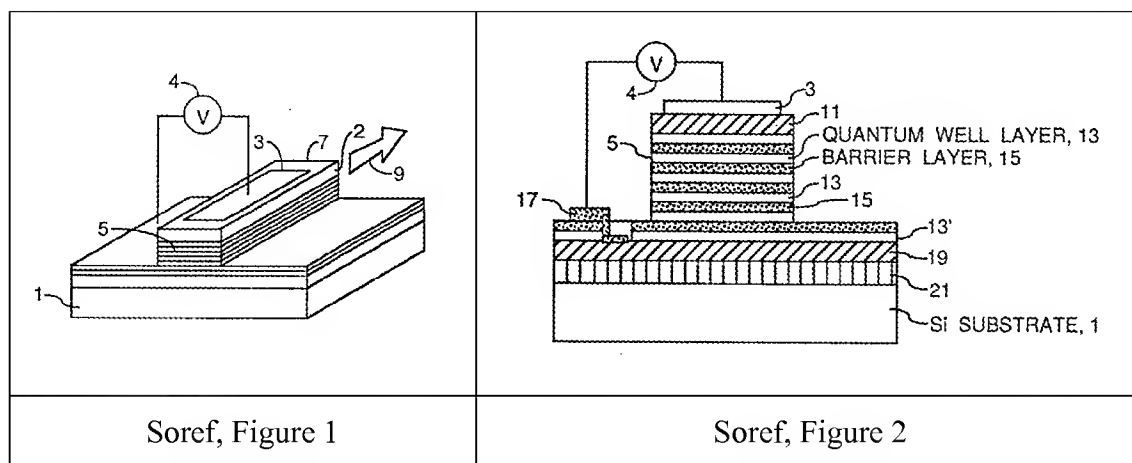
(i) a single graded layer containing Si, Ge, and Sn, whose composition is "Si-like" at the Si substrate and "GeSn-like" at the active layer (#13'); or

(ii) or two separate buffer layers, one graded from pure Si to pure Ge (#21) and the second graded from pure Ge to $Ge_{0.95}Sn_{0.05}$.

Neither alternative describes the presently claimed essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer.

Additionally, for Soref to anticipate instant claim 9, it must also disclose the combination of the constituent elements; that is, a Sn_zGe_{1-z} layer formed over a substrate, and an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer. In the present rejection, the Office alleges that Soref teaches, according to the numbering in Figures 1 and 2 of Soref,

> *"a substrate (Soref figs. 1 or 2 #1), a Sn_zGe_{1-z} layer formed over the substrate (Soref figs 1 or 2 #13 col. 2 line 45-47), and an essentially single-phase $Ge_{1-x-y}Sn_xSi_y$ layer formed over the Sn_zGe_{1-z} layer (Soref figs. 1 or 2 #19, col. 3 line 44-45)."*

For convenience, Figures 1 and 2 of Soref read as follow:
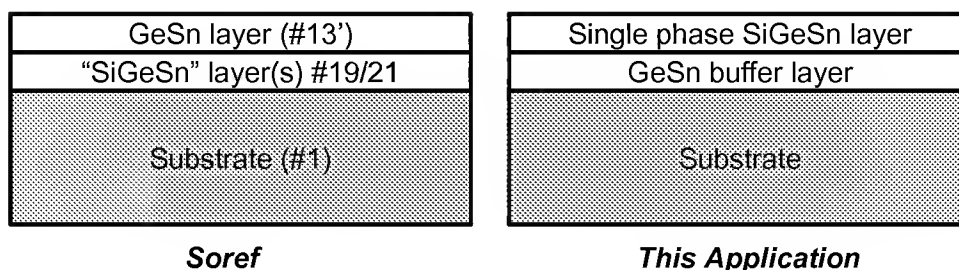
| Soref, Figure 1 | Soref, Figure 2 |

where individual components are (see Column 2, Lines 41 – 58): **3** – ohmic contact **4** – current source; **5** – reflective end facet; **11** – relaxed upper buffer layer (p- or n-doped, see Col. 4, Lines 19 – 23); **13** – GeSn quantum wells (QW); **13'**- 'active QW layer'; **15** – barrier layers; **17** – ohmic contact; **19** – n-doped buffer layer; and **21** - n-doped buffer layer.

Applicants note that according to Figure 2, layer #19 (a spatially graded buffer layer of "SiGeSn"; see, Col. 3, lines 25 - 29) is formed over the substrate *(layer #1)*, and layer #13 (a GeSn quantum well; see, Col. 2, lines 45 – 46) is formed over layer #19. The only layer shown between the "SiGeSn layer" (#19) and the substrate (#1) is layer #21, not layer #13 as alleged by the Office.

Layer #21 is the "lower buffer layer" which is described as *"relaxed SiGe with a composition that varied between pure Si and pure Ge"* (see Col. 3, ll. 33 – 44, *supra*). Accordingly, Soref teaches a *graded* "SiGeSn layer" (layer #19) formed over the substrate (layer #1) with a GeSn layer (layer #13) formed over the "SiGeSn" layer.

The differences between Soref can be readily seen in the following figure, in Soref, the GeSn layer is formed on top of the "SiGeSn" layer while in the instant application and claims, the GeSn layer is formed on the substrate and provides for the formation of the SiGeSn thereover.

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GeSn layer (#13')		Single phase SiGeSn layer
"SiGeSn" layer(s) #19/21		GeSn buffer layer
Substrate (#1)		Substrate

| Soref | This Application |

The combination of layers disclosed in Soref is not the same as produced the instantly claimed method of Claim 9. Applicants submit that Soref describe neither the instantly claimed essentially single-phase SiGeSn layer nor the proper order of layers in the presently claimed structures, and therefore, the Office has failed to establish a *prima facie* case for anticipation of instant Claim 9.

Applicants maintain that the "essentially single phase" SiGeSn layer of Claim 9 is neither explicitly or inherently anticipated by Soref, nor is the presently claimed structure described. However, even *if* the Office maintains that the "essentially single phase" SiGeSn layer **and** a method for producing the combination of layers in the presently claimed structures are disclosed, Applicants submit that Soref is not enabling for such compositions comprising an essentially single phase SiGeSn layer.

"In determining that quantum of prior art disclosure which is necessary to declare an applicant's invention 'not novel' or 'anticipated' within section 102, the stated test is whether a reference contains an 'enabling disclosure'... ." *In re Hoeksema,* 399 F.2d 269, 158 USPQ 596 (CCPA 1968). The disclosure in an assertedly anticipating reference must provide an enabling disclosure of the desired subject matter; mere naming or description of the subject matter is insufficient, if it cannot be produced without undue experimentation. *Elan Pharm., Inc. v. Mayo Found. For Med. Educ. & Research,* 346 F.3d 1051, 1054, 68 USPQ2d 1373, 1376 (Fed. Cir. 2003). MPEP 2121.01. Where a process for making the compound is not developed until after the date of invention, the mere naming of a compound in a reference, without more, cannot constitute a description of the compound. *In re Hoeksema,* 399 F.2d 269, 158 USPQ 596 (CCPA 1968). MPEP 2121.02(I). (Emphasis added)

As stated in the present specification, at the time of filing, the presently claimed SiGeSn compositions were experimentally unknown and their properties only had been investigated by

theoretical means (see, Specification, paragraph [0007]). The instant application describes for the first time, a method for preparing such a SiGeSn compositions (see, Specification, [0010]).

The synthetic methods mentioned in Soref are chemical vapor deposition (CVD) and molecular beam epitaxy (MBE) (see, Col. 2, lines 11 – 19). Upon or review, it does not appear that Soref contains any further discussion of the preparation of any of the layers. Applicants note that the discussion at Col. 2, lines 11 – 19 is related to **GeSn** layers and not any "SiGeSn" layer:

> *The active material here is a **germanium-tin** alloy. Experiments have been reported in the literature where several percent of alpha-tin (as much as 25%) were incorporated in a germanium lattice by means of "epitaxial stabilization" which is a form of non-equilibrium growth. The growth techniques are chemical vapor deposition (CVD) and molecular beam epitaxy (MBE). The growth procedures are similar to those used for $Si_{1-x}Ge_x$ upon Si, thus the **GeSn growth** is expected to be quite feasible.*

Soref is silent with respect to any methods for preparing any "SiGeSn layer", regardless of whether it is graded or a single phase.

Therefore, at the time of filing the instant application, one skilled in the art, given the Soref reference, would require undue experimentation to prepare the claimed essentially single-phase SiGeSn layers, as evidenced by the substantial lack of known methods for preparing the same in the art. Without a proper description of how to make the claimed essentially single phase SiGeSn layer, and without the knowledge available in the art, one skilled in the art would not be able to make the claimed essentially single phase SiGeSn layer based solely on the Soref reference. For example, MPEP 2121.02, "Compounds and compositions – What Constitutes Enabling Prior Art", states in relevant portions,

> *I.< ONE OF ORDINARY SKILL IN THE ART MUST BE ABLE TO MAKE OR SYNTHESIZE*
>
> *Where a process for making the compound is not developed until after the date of invention, the mere naming of a compound in a reference, without more, cannot constitute a description of the compound. In re Hoeksema, 399 F.2d 269, 158 USPQ 596 (CCPA 1968). Note, however, that a reference is presumed operable until applicant provides facts rebutting the presumption of *>operability<. In re Sasse, 629 F.2d 675, 207 USPQ 107 (CCPA 1980). Therefore, applicant must provide evidence showing that a process for making was not known at the time of the invention. See the following paragraph for the evidentiary standard to be applied.*

> *II.< A REFERENCE DOES NOT CONTAIN AN "ENABLING DISCLOSURE" IF ATTEMPTS AT MAKING THE COMPOUND OR COMPOSITION WERE UNSUCCESSFUL BEFORE THE DATE OF INVENTION*

When a prior art reference merely discloses the structure of the claimed compound, evidence showing that attempts to prepare that compound were unsuccessful before the date of invention will be adequate to show inoperability. In re Wiggins, 488 F.2d 538, 179 USPQ 421 (CCPA 1971).

In support of Applicants assertion that the presently claimed materials were experimentally unknown at the time of filing of the instant application, Applicants refer to Aella, *et al. Appl. Phys. Lett.* **2004**, *84*, 888, which states in the first paragraph in the left-hand column of page 888, "*Our own prelimary study describes the first successful growth of this material [Si-Ge-Sn]*," referencing Bauer *et al., Appl. Phys. Lett.* **2003**, *83*, 2163. Copies of both Aella and Bauer are included in Section IX of this Appeal Brief. Both peer-reviewed references illustrate that it was accepted in the art, after filing of the instant application, that methods for making the instantly claimed materials were unknown until the instant invention thereof.

For the preceding reasons, Applicants submit the instant rejection of claim 9 as anticipated by Soref is improper and respectfully request reconsideration and withdrawal of the rejection.

3. Independent Claim 19

In the present Final Office Action, the Office has alleged that claim 19 is anticipated by Soref, and cited the same support as for independent Claim 1 (*supra*).

Claim 19 presently reads,

19. (Previously presented) An alloy of the formula, $Ge_{1-x-y}Si_xSn_y$, wherein x is about 0.01 to about 0.25 and y is about 0.01 to about 0.11.

As previously noted with respect to the outstanding rejection of Claim 1, upon review of Soref, Applicants note that "SiGeSn" materials are discussed in Soref in the Abstract, at Column 3, lines 25 – 29, at Column 3, lines 33 – 44, and Claim 16 (*supra*). Applicants note that Soref describes buffer layers (layers #19 and 21, Figure 2) between a substrate (#1) and "active quantum wells" containing GeSn (#13') as a "SiGeSn layer" (see, Figure 2 and Col. 2, ll. 52 – 55). The buffer layers "can be constructed from a spatially varying (graded) composition alloy of SiGeSn" (see, Col. 3, ll. 25 – 27). A definition for a "varying (graded) composition alloy of SiGeSn" follows at Col. 3, lines 27 – 29, "*At the Si wafer, the buffer layer 21 is Si-like. At the top surface of the buffer layer 19, the alloy is like GeSn, for example, $Ge_{0.92}Sn_{0.08}$.*"

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Applicants note that Soref describes buffer layers (layers #19 and 21, Figure 2) between a substrate (#1) and "active quantum wells" containing GeSn (#13') as a "SiGeSn layer" (see, Figure 2 and Col. 2, ll. 52 – 55). The buffer layers "can be constructed from a spatially varying (graded) composition alloy of SiGeSn" (see, Col. 3, ll. 25 – 27). A definition for a "varying (graded) composition alloy of SiGeSn" follows at Col. 3, lines 27 – 29, *"At the Si wafer, the buffer layer 21 is Si-like. At the top surface of the buffer layer 19, the alloy is like GeSn, for example, $Ge_{0.92}Sn_{0.08}$."*

Soref is merely using the term "SiGeSn layer" to refer to graded compositions which satisfy the stated compositions at the faces of layers #19 and #21. Such materials are not the presently claimed SiGeSn alloys.

Further, Soref acknowledges, *"It may be difficult technically to grade the composition of the SiGeSn lower buffer from pure silicon up to germanium-tin"* (see, Col. 3, ll. 36 – 38). As an alternative, Soref suggests the use of two separate layers (i.e., layers #19 and #21), which themselves are also graded compositions, *"In that case, two buffer layers can be grown upon the silicon substrate: for example, lower buffer layer 21 could be relaxed SiGe, with a composition that varied between pure Si and pure Ge; and lower buffer 19 would be a relaxed alloy of GeSn, whos composition varied from pure Ge to $Ge_{0.95}Sn_{0.05}$"* (see, Col. 3, ll. 38 – 44).

Therefore, for the buffer layer (#19) between the substrate (#1) and the active GeSn layer (#13)' Soref describes the use of either

(i) a single graded layer containing Si, Ge, and Sn, whose composition is "Si-like" at the Si substrate and "GeSn-like" at the active layer (#13'); or

(ii) or two separate buffer layers, one graded from pure Si to pure Ge (#21) and the second graded from pure Ge to $Ge_{0.95}Sn_{0.05}$.

Neither alternative describes the presently claimed alloys of $Ge_{1-x-y}Si_xSn_y$, where x is about 0.01 to about 0.25 and y is about 0.01 to about 0.11. Nowhere does Soref describe a "SiGeSn" layer or material where all three constituent elements are simultaneously present in a form which may be called a SiGeSn alloy, and particularly, not together in the presently claimed alloy compositional ranges.

The Office has further alleged on page 6 through 7 of the Final office action (emphasis original),

> *The layer [SiGeSn layer] <u>can be constructed</u>...i.e. the strained layer can be spatially varying or not spatially varying and in the embodiment wherein the strained is not spatially varying applicants' arguments are not persuasive.*

> *It is noted that it is readily apparent to one skilled in the art that Soren's [sic] uses the same material for the same material (Si-Ge-Sn) alloy for the same purpose (strain free layers) therefore what is true for Applicant's (Si-Ge-Sn alloys are particularly suitable to form highly uniform (i.e. substantiall single phase) is also true for Soren [sic]. Further Applicants' specification para 0032 states (in relevant parts) "materials like Si-ge-Sn alloys are chosen because they form highly uniform layers , all of which make it clear to one of ordinary skill in the art , that Soren [sic] also discloses its layer to be highly uniform i.e. consists elemental uniformity of material that is consistent with single phase alloy layer.*

The Office has raised two issues here; one appears to invoke an alleged inherent disclosure of the presently claimed $Ge_{1-x-y}Si_xSn_y$ alloys; and the second is an alleged admission by Applicants regarding the nature of SiGeSn alloys. On each point, Applicants respectfully submit that the Office is incorrect.

First, Applicants submit that the Office has not met its burden of proof to establish that the missing descriptive matter (*i.e.*, a non-graded "SiGeSn" layer or material) is necessarily present in Soref to support a rejection based on an alleged inherent teaching. As stated in *Ex Parte Levy, 17 USPQ2d, 1461, 1464 (citing In re King, 801 F.2d 1324), "In relying upon the theory of inherency, the examiner must provide a basis in fact and/or technical reasoning to reasonable support the determination that the alledgedly inherent characteristic necessarily flows from the prior art."*

Analagous to *Ex Parte Levy* (as discussed previously), Soref does not mention a SiGeSn alloy, only graded compositions (*supra*). Further, Soref does not provide any working examples, or any other discussion for that matter, revealing the process conditions employed to produce any "SiGeSn" alloy. The Office has not offered any evidence to provide a basis in fact and/or technical reasoning that a SiGeSn alloy necessarily flows from the teachings of Soref.

In the second point, Applicants submit that paragraph [0032] of the instant specification has nothing to do with the SiSnGe alloys as asserted and relied upon by the Office. The referenced paragraph of the specification reads, in whole, (emphasis added),

*We initially investigated the growth of $Si_{1-x-y}Ge_xSn_y$ directly on Si(100) using $Ge_{1-x}Sn_x$ (x=2-4 at. %) buffer layers. We chose **$Ge_{1-x}Sn_x$ alloys** as buffer layers because they possess crystallographic, morphological and mechanical properties that make them uniquely suitable for use as templates on Si substrates. **These materials** grow as highly uniform, strain-free layers with smooth and continuous surface morphologies (typical AFM rms values are 0.5 and 1.4 nm) and display extremely low concentrations of threading defects, particularly those that extend to the uppermost surface (the quality of pure Ge films grown on Si by similar methods is much worse). In addition, **they** are high compressibility (softer) solids compared to either Si and $Si_{1-x-y}Ge_xSn_y$ and thereby **can act as potential spacers** that can conform structurally and readily absorb the differential strain imposed by the more rigid Si and Si-Ge-Sn.*

Rather paragraph [0032] is wholly concerned with the $Ge_{1-x}Sn_x$ buffer layer (note the comparisons to SiGeSn in the final sentence). In fact, Applicants have been unable to find any statement in the instant specification which contains, *"materials like Si-Ge-Sn alloys are chosen because they form highly uniform layer..."* as quoted by the Office in the present action. Thus, Applicants have not admitted, and do not admit, that *"Si-Ge-Sn alloys are chosen because they form highly uniform layer,"* in fact, such a statement would have been impossible by Applicants as the Si-Ge-Sn alloys were experimentally unknown prior to the instant invention (see, Specification, paragraphs [0007] and [0010]).

While Applicants maintain that the SiGeSn alloy of Claim 19 is neither explicitly or inherently anticipated by Soref, even *if* the Office maintains that the SiGeSn alloy is disclosed, Applicants further submit that Soref is not enabling for such SiGeSn alloys.

"In determining that quantum of prior art disclosure which is necessary to declare an applicant's invention 'not novel' or 'anticipated' within section 102, the stated test is whether a reference contains an 'enabling disclosure'... ." *In re Hoeksema,* 399 F.2d 269, 158 USPQ 596 (CCPA 1968). The disclosure in an assertedly anticipating reference must provide an enabling disclosure of the desired subject matter; mere naming or description of the subject matter is insufficient, if it cannot be produced without undue experimentation. *Elan Pharm., Inc. v. Mayo Found. For Med. Educ. & Research,* 346 F.3d 1051, 1054, 68 USPQ2d 1373, 1376 (Fed. Cir. 2003). MPEP 2121.01. Where a process for making the compound is not developed until after the date of invention, the mere naming of a compound in a reference, without more, cannot constitute a description of the compound. *In re Hoeksema,* 399 F.2d 269, 158 USPQ 596 (CCPA 1968). MPEP 2121.02(I). (Emphasis added)

As stated in the present specification, at the time of filing, the presently claimed SiGeSn compositions were experimentally unknown and their properties only had been investigated by theoretical means (see, Specification, paragraph [0007]). The instant application describes for the first time, a method for preparing such a SiGeSn compositions (see, Specification, [0010]).

The synthetic methods mentioned in Soref are chemical vapor deposition (CVD) and molecular beam epitaxy (MBE) (see, Col. 2, lines 11 – 19). Upon or review, it does not appear that Soref contains any further discussion of the preparation of any of the layers. Applicants note that the discussion at Col. 2, lines 11 – 19 is related to **GeSn** layers and not any "SiGeSn" layer:

> *The active material here is a **germanium-tin** alloy. Experiments have been reported in the literature where several percent of alpha-tin (as much as 25%) were incorporated in a germanium lattice by means of "epitaxial stabilization" which is a form of non-equilibrium growth. The growth techniques are chemical vapor deposition (CVD) and molecular beam epitaxy (MBE). The growth procedures are similar to those used for $Si_{1-x}Ge_x$ upon Si, thus the **GeSn growth** is expected to be quite feasible.*

Soref is silent with respect to any methods for preparing any "SiGeSn layer", regardless of whether it is graded or an alloy.

Therefore, at the time of filing the instant application, one skilled in the art, given the Soref reference, would require undue experimentation to prepare the claimed SiGeSn alloys, as evidenced by the substantial lack of known methods for preparing the same in the art. Without a proper description of how to make the claimed alloys, and without the knowledge available in the art, one skilled in the art would not be able to make the claimed SiGeSn alloys based solely on the Soref reference. For example, MPEP 2121.02, "Compounds and compositions – What Constitutes Enabling Prior Art", states in relevant portions,

> *I.< ONE OF ORDINARY SKILL IN THE ART MUST BE ABLE TO MAKE OR SYNTHESIZE*
> *Where a process for making the compound is not developed until after the date of invention, the mere naming of a compound in a reference, without more, cannot constitute a description of the compound. In re Hoeksema, 399 F.2d 269, 158 USPQ 596 (CCPA 1968). Note, however, that a reference is presumed operable until applicant provides facts rebutting the presumption of *>operability<. In re Sasse, 629 F.2d 675, 207 USPQ 107 (CCPA 1980). Therefore, applicant must provide evidence showing that a process for making was not known at the time of the invention. See the following paragraph for the evidentiary standard to be applied.*

II.< A REFERENCE DOES NOT CONTAIN AN "ENABLING DISCLOSURE" IF AT-TEMPTS AT MAKING THE COMPOUND OR COMPOSITION WERE UNSUCCESSFUL BEFORE THE DATE OF INVENTION

When a prior art reference merely discloses the structure of the claimed compound, evidence showing that attempts to prepare that compound were unsuccessful before the date of invention will be adequate to show inoperability. In re Wiggins, 488 F.2d 538, 179 USPQ 421 (CCPA 1971).

In support of Applicants assertion that the presently claimed materials were experimentally unknown at the time of filing of the instant application, Applicants refer to Aella, *et al. Appl. Phys. Lett.* **2004**, *84*, 888, which states in the first paragraph in the left-hand column of page 888, *"Our own prelimary study describes the first successful growth of this material [Si-Ge-Sn],"* referencing Bauer *et al., Appl. Phys. Lett.* **2003**, *83*, 2163. Copies of both Aella and Bauer are included in Section IX of this Appeal Brief. Both peer-reviewed references illustrate that it was accepted in the art, after filing of the instant application, that methods for making the instantly claimed materials were unknown until the instant invention thereof.

Accordingly applicants submit that the present rejection of claim 19 is improper, and respectfully request reconsideration and withdrawal of the rejection.

4. Independent Claim 27

In the present Final Office Action. the Office has alleged that claim 27 is anticipated by Soref, and cited the same support as for independent Claims 1 and 19 (*supra*).

Claim 27 presently reads,

27. (Previously presented) A structure comprising: a Sn_zGe_{1-z} layer and a layer of the alloy of Claim 19 formed over the Sn_zGe_{1-z} layer.

As previously noted with respect to the outstanding rejection of Claim 19, Applicants submit that Soref does not teach the presently claimed layer of an $Ge_{1-x-y}Si_xSn_y$ alloy. wherein x is about 0.01 to about 0.25 and y is about 0.01 to about 0.11.

Additionally, for Soref to anticipate instant claim 27, it must also disclose the recited combination of the constituent elements; that is, the $Ge_{1-x-y}Si_xSn_y$ alloy layer formed over a Sn_zGe_{1-z} layer. In the present rejection, the Office alleges that Soref teaches, according to the numbering in Figures 1 and 2 of Soref,

"a substrate (Soref figs. 1 or 2 #1), a Sn_zGe_{1-z} layer formed over the substrate (Soref figs 1 or 2 #13 col. 2 line 45-47), and an essentially single-phase $Ge_{1-x-y}Sn_xSi_y$ layer formed over the Sn_zGe_{1-z} layer (Soref figs. 1 or 2 #19, col. 3 line 44-45)."

Applicants note that according to Figure 2, layer #19 (a spatially graded buffer layer of "SiGeSn"; see, Col. 3, lines 25 - 29) is formed over the substrate *(layer #1)*, and layer #13 (a GeSn quantum well; see, Col. 2, lines 45 – 46) is formed over layer #19. The only layer shown between the "SiGeSn layer" (#19) and the substrate (#1) is layer #21, <u>not layer #13</u> as alleged by the Office.

Layer #21 is the "lower buffer layer" which is described as *"relaxed SiGe with a composition that varied between pure Si and pure Ge"* (see Col. 3, ll. 33 – 44, *supra*). Accordingly, Soref teaches a *graded* "SiGeSn layer" (layer #19) formed over the substrate (layer #1) with a GeSn layer (layer #13) formed over the "SiGeSn" layer.

The combination of layers disclosed in Soref is not the same as the instantly claimed arrangement. Further, as Soref does not describe the alloys according to claim 19 (supra), it cannot teach such an alloy layer over any other layer.

To establish a *prima facie* case for anticipate Claim 27 by Soref, Soref must expressly or inherently disclose the claimed composition and combination of layers. Applicants submit that Soref describe neither the instantly claimed SiGeSn alloy layer nor the proper order of layers in the presently claimed structures, and therefore, the Office has failed to establish a *prima facie* case for anticipation of instant Claim 27.

While Applicants maintain that the SiGeSn alloy layer of Claim 27 is neither explicitly or inherently anticipated by Soref, nor is the presently claimed structure described, even *if* the Office maintains that the SiGeSn alloy layer **and** the combination of layers in the presently claimed structures are disclosed, Applicants submit that Soref is not enabling for such compositions comprising a SiGeSn alloy layer.

As stated in the present specification, at the time of filing, the presently claimed SiGeSn compositions were experimentally unknown and their properties only had been investigated by theoretical means (see, Specification, paragraph [0007]). The instant application describes for the first time, a method for preparing such a SiGeSn compositions (see, Specification, [0010]).

Applicants refer to their preceding discussion of enablement with respect to Claim 19. In

sum, Soref is **_silent_** with respect to any methods for preparing any "SiGeSn layer", regardless of whether it is graded or a single phase. In support of Applicants assertion that the presently claimed materials were experimentally unknown at the time of filing of the instant application, Applicants refer to Aella, *et al. Appl. Phys. Lett.* **2004**, *84*, 888 ('Aella'), which states in the first paragraph in the left-hand column of page 888, *"Our own preliminary study describes the first successful growth of this material [Si-Ge-Sn],"* referencing Bauer *et al., Appl. Phys. Lett.* **2003**, *83*, 2163 ('Bauer'). Both Aella[4] and Bauer[5] were introduced as evidence in the instant application in the Information Disclosure Statement, filed by Applicant on December 8, 2006. Each was considered and entered into the record by the examiner by their consideration on March 2, 2007. Copies of both Aella and Bauer are included in Section IX of this Appeal Brief. Both peer-reviewed references illustrate that it was accepted in the art, at the time of filing of the instant application that methods for making the instantly claimed materials were unknown until the instant invention thereof. Aella published on February 9, 2004 and Bauer published on September 15, 2003.

For each of the preceding reasons, that Soref does not explicitly or inherently disclose a SiGeSn alloy layer as presently claimed nor explicitly or inherently disclose the claimed combination of layers; and that Soref is not enabled for any method for preparing the instantly claimed SiGeSn alloy layers, Applicants submit that Soref does not anticipate Claim 27. Applicants respectfully request reconsideration and withdrawal of the rejection.

5. Dependent Claims

Applicants make the following observations regarding deficiencies in the disclosure of Soref with respect to the dependent claims. Applicants submit the rejections each of dependent claims are improper for failing to anticipate all the claimed limitations.

a. Dependent Claims 4 - 6, 14 – 16, and 20 - 22

The Office has alleged that claims 4 – 6 are anticipated by Soref, and cited Col. 2, line 39; Col. 2, lines 60 – 65; Col. 3, lines 29 and 44; the abstract, and Claim 16 therein. Claims 4 – 6 are dependent on Claim 1, and are directed to semiconductor structures comprising: a substrate,

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[4] See Document No. 75

[5] See Document No. 70

a Sn_zGe_{1-z} layer formed over the substrate, and an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer with further limitations related to variables 'x', 'y', and 'z'. Namely, Claim 4 recites the structure of claim 1, wherein z is about 0.01 to about 0.05; Claim 5 recites the structure of claim 1, wherein x is about 0.01 to about 0.25; and y is about 0.01 to about 0.11; and Claim 6 recites the structure of claim 1, wherein x is about 0.01 to about 0.25; y is about 0.01 to about 0.11; z is about 0.01 to about 0.05; and the substrate comprises silicon.

The Office has alleged that claims 14 – 16 are anticipated by Soref, and cited the same passages as for claims 4 - 6. Claims 14 – 16 are dependent on Claim 9, and are directed to methods to prepare a semiconductor structure comprising: a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and an $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer (i.e., essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer of Claim 1) with the further limitations related to variables 'x', 'y', and 'z'. Namely, Claim 14 recites the method of claim 9, wherein z is about 0.01 to about 0.05; Claim 15 recites the method of claim 9, wherein x is about 0.01 to about 0.25; and y is about 0.01 to about 0.11; and Claim 16 recites the method of claim 9, wherein x is about 0.01 to about 0.25; y is about 0.01 to about 0.11; z is about 0.01 to about 0.05; and the substrate comprises silicon.

The Office has alleged that claims 20 – 22 are anticipated by Soref, and cited the same passages as for claims 4 - 6. Claims 20 – 22 are dependent on Claim 19, and are directed to alloys of the formula, $Ge_{1-x-y}Si_xSn_y$, with further limitations related to variables 'x' and 'y'. Namely, Claim 20 recites alloy of Claim 19, wherein x is about 0.13 to about 0.20; claim 21 recites the alloy of Claim 20, wherein y is about 0.07 to about 0.11; and claim 22 recites the alloy of Claim 20, wherein y is about 0.01 to about 0.06.

With respect to the passages cited in Soref by the Office, Applicants note that each citation reads:

Col. 2, line 39:

> ...*300 Å barriers of* $Ge_{.85}Se_{.15}$. *This theory supports the...*

Col. 2, lines 60 – 65:

> *Theory indicates the multiple quantum well (MWQ) directness or direct gap will exist for a range of compositions: for example, 2% to 15% tin in the wells, with the barriers having a composition of 3% to 6% more tin than the percent Sn in the wells.*

The parameters in FIG. 2 are as follows: x is less than y; s is about 0.1 and z is about 0.5(x+y).

Col. 3, line 29:

...GeSn, for example, $Ge_{0.92}Sn_{0.08}$. This buffer is doped n-type,...

Col. 3, line 44:

...pure Ge to $Ge_{0.95}Sn_{0.05}$. Both lower buffers could be doped...

the Abstract (emphasis added):

> *Silicon-based laser diodes, optical amplifiers, electrooptical modulators, and photodetectors in which the active region consists of a pseudomorphic GeSn multiple quantum well stack. Each quantum well is tensile-strained $Ge_{1-x}Sn_x$ layer sandwiched between compressively strained barriers of $Ge_{1-y}Sn_y$, with x-0.1, x<y and y=0.15. The GeSn quantum wells have a strain-induced direct gap for strongly allowed band-to-band transitions in the infrared range.* **The quantum well stack is grown upon a relaxed SiGeSn alloy buffer portion whose composition is graded up from a lattice match at the silicon substrate interface to a Ge or GeSn composition at buffer's top surface.** *Doped cladding layers are added, so that the devices have a p-i-n diode structure. The monolithic integrated Column IV devices have a rib waveguide structure, where desired, and operate typically in the 2 to 3 micron wavelength range.*

and Claim 16 therein (emphasis added):

> *16. A semiconductor optical device comprising:*
> *(a) an active region made up of a multiple quantum well stack having in-plane tensile strained germanium-tin alloy quantum wells and germanium-tin alloy barriers, said quantum well stack having given lattice constants, and wherein the quantum wells have an atomic percentage of tin of 5% to 15%, enabling a direct bandgap to exist between the n=1 conduction subband and the n=1 valence subband of the multiple quantum wells of said stack and wherein said barriers have an atomic percentage of tin of 3% to 6% more than the percentage of tin in the quantum wells and are compressively strained in-plane for producing symmetric strain for the quantum well stack to enable a thick high quality stack to be formed;*
> *(b) a doped relaxed SiGeSn **graded composition** lower buffer portion positioned below the stack, grown upon and contacting a substrate selected from the group consisting of Si and Ge;*
> *(c) a doped relaxed GeSn composition upper buffer portion positioned above the stack, and wherein said upper and lower buffer layers each have a zincblend lattice constant that is halfway between the lattice constant of the wells and the lattice constant of the barriers; and*
> *(d) a first electrode coupled to said upper buffer layer portion and a second electrode coupled to said lower buffer layer portion.*

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With respect to the passages in Soref cited by the Office, Applicants note that,

Col. 2, line 39 relates to **GeSn** barriers ($Ge_{0.85}Sn_{0.15}$; *i.e.*, z = 0.15);

Col. 2, lines 60 - 65 relates to **GeSn** quantum wells (see, Col. 2, lines 45 – 47);

Col. 3, line 29 relates to **GeSn** barriers ($Ge_{0.92}Sn_{0.08}$; *i.e.*, z = 0.08);

Col. 3, line 44 relates to **GeSn** barriers ($Ge_{0.95}Sn_{0.05}$; *i.e.*, z = 0.05);

the Abstract relates to **graded** "SiGeSn compositions"; and

Claim 16 relates to **graded** "SiGeSn compositions."

Thus, none of these citations relied upon by the Office for establishing that Soref anticipates the present dependent claims provides any teaching regarding an essentially single phase SiGeSn, a SiGeSn alloy, or any of the specific limitations recited in the dependent claims.

In combination with the previous discussions of independent claims 1, 9 and 19, as Soref does not describe, explicitly or inherently, the presently claimed SiGeSn layers, alloys, nor enables any methods for their preparation, neither are the particular limitations of instant Claims 4 – 6, 14 – 16, and 20 – 22 anticipated by Soref.

b. Dependent Claims 7 – 8

The Office has alleged that claims 7 - 8 are anticipated by Soref, and cited the Abstract (*supra*) therein. Claims 7 - 8 are dependent on Claim 1, and are directed to semiconductor structures comprising: a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer with the further limitations that the $Ge_{1-x-y}Si_xSn_y$ layer is **strained** (Claim 7) or **relaxed** (Claim 8). Applicants note that the Abstract mentions that the "SiGeSn layer" in Soref is both relaxed **and** graded (see Abstract, lines 8 – 12) and is silent with respect to strained SiGeSn layers.

Soref discusses strain in the *multiple quantum well* layers therein at Col. 2, l. 59 – Col. 3, l. 24:

> *Theory indicates the multiple quantum well (MWQ) directness or direct gap will exist for a range of compositions: for example, 2% to 15% tin in the*

*wells, with the barriers having a composition of 3% to 6% more tin than the percent Sn in the wells. The parameters in FIG. 2 are as follows: x is less than y; x is about 0.1 and z is about 0.5(x+y). These compositions produce barriers with a wider gap than the wells, and the strained layer superlattice is Type I. The GeSn tensile wells are tensile-strained in plane. There are two possibilities for strain in the barrier layers 15: unstrained, or compressively strained barriers. Usually, we prefer strain that is equal, but opposite sign, in the wells and barriers. This is called symmetric strain for the quantum stack. In that case, the **buffer layer upon which the MQW stack is grown should have a zincblende lattice parameter that is halfway between the lattice constant of the wells and the lattice constant of the barriers.** Symmetric strain allows a thick high-quality stack to be grown. The thickness of individual layers is chosen to be less than the critical layer thickness for stable strain, which gives monocrystal layers with very few misfit dislocations per cm. sq.*

We choose to call the MQW stack pseudomorphic" because all layers are coherently strained with near-perfect crystal quality (low defect density).

The in-plane lattice size of the wells and barriers conforms to the lattice size of the buffer. Thus, the buffer's lattice size is "reproduced" throughout the stack. *This is called commensurate growth or coherent strain. Strain is produced in the epitaxial layers by the mismatch between the buffer lattice parameter and the well-or-barrier lattice that would of existed in a bulk alloy crystal. The bulk lattice size is determined by the Ge/Sn ratio (the alloy composition).*

While Soref does discuss matching the "lattice size" of the buffer layer (layer #19, Figure 2) to the MQW stack layers and the strain produced in each as a result, the buffer layer described in Soref is not the presently claimed "essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer."

Accordingly, Soref does not explicitly or inherently anticipate a strained or relaxed essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer nor the same layer in the presently claimed structure.

c. Dependent Claim 10

The Office has alleged that claim 10 is anticipated by Soref, and cited Col. 2, lines 15 - 20 therein.   Claim 10 is dependent on Claim 9, and is directed to a method to prepare a semiconductor structure comprising: a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and an $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer (i.e., essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer of Claim 1) formed over the Sn_zGe_{1-z} layer with the further limitation that the $Ge_{1-x-y}Si_xSn_y$ layer is deposited by precursor chemical vapor deposition, wherein the precursor chemical vapor comprises **SnD$_4$ and H$_3$SiGeH$_3$**.

Applicants note that the neither the claimed reagents individually (*i.e.*, SnD_4 and H_3SiGeH_3) nor the claimed combination, much less their use in a method for the preparation of SiGeSn layers, appear in Soref. The Office has offered no evidence of record that the use of the presently claimed species for the deposition of an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer by precursor chemical vapor deposition was known, to one skilled in the art, at the time of filing of the instant application. Accordingly, Soref does not explicitly anticipate the claimed method.

Further, Soref is ___*silent*___ with respect to any additional methods for preparing any SiGeSn layers. The Office has not made any evidence of record to establish that, at the time of filing of the instant application, any methods were known to those skilled in the art for preparing a SiGeSn alloy of the claimed compositional ranges, nor made any evidence of record teaching one skilled in the art to use the particularly claimed combination of reagents. Applicants submit that the Office has not met its burden of proof to establish that the missing descriptive matter (*i.e.*, a non-graded SiGeSn layer) is necessarily present in Soref to support a rejection based on an alleged inherent teaching.

Accordingly, Soref does not disclose, explicitly or inherently, the presently claimed methods for preparing SiGeSn layer.

d. Dependent Claim 11

The Office has alleged that claim 11 is anticipated by Soref, and cited Col. 2 therein. Claim 11 is dependent on Claim 9, and is directed to a method to prepare a semiconductor structure comprising: a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and an $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer (i.e., essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer of Claim 1) formed over the Sn_zGe_{1-z} layer with the further limitation that the Sn_zGe_{1-z} layer is deposited by precursor chemical vapor deposition, wherein the precursor chemical vapor comprises __SnD_4 and Ge_2H_6__.

Applicants note that the neither the claimed reagents individually (*i.e.*, SnD_4 and Ge_2H_6) nor the claimed combination thereof, much less their use in a method for the preparation of SiGeSn layers, appear in Soref. The Office has offered no evidence of record that the use of the presently claimed species for the deposition of an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer by

precursor chemical vapor deposition was known, to one skilled in the art, at the time of filing of the instant application. Accordingly, Soref does not explicitly anticipate the claimed method.

Further, Soref is **_silent_** with respect to methods for preparing any SiGeSn layers. The Office has not made any evidence of record to establish that, at the time of filing of the instant application, any methods were known to those skilled in the art for preparing the claimed SiGeSn layers, nor made any evidence of record teaching one skilled in the art to use the particularly claimed combination of reagents. Applicants submit that the Office has not met its burden of proof to establish that the missing descriptive matter (*i.e.*, a non-graded SiGeSn layer) is necessarily present in Soref to support a rejection based on an alleged inherent teaching.

Accordingly, Soref does not disclose, explicitly or inherently, the presently claimed methods for preparing SiGeSn layer.

e. Dependent Claim 25

The Office has alleged that claim 25 is anticipated by Soref, and cited the Examples therein. Claim 25 is dependent on Claim 1, and is directed to a semiconductor structure comprising: a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer with the further limitation that the Sn_zGe_{1-z} and $Ge_{1-x-y}Si_xSn_y$ layers are **lattice-matched**.

Soref discusses strain in the *multiple quantum well* layers therein at Col. 2, l. 59 – Col. 3, l. 24:

> *Theory indicates the multiple quantum well (MWQ) directness or direct gap will exist for a range of compositions: for example, 2% to 15% tin in the wells, with the barriers having a composition of 3% to 6% more tin than the percent Sn in the wells. The parameters in FIG. 2 are as follows: x is less than y; x is about 0.1 and z is about 0.5(x+y). These compositions produce barriers with a wider gap than the wells, and the strained layer superlattice is Type I. The GeSn tensile wells are tensile-strained in plane. There are two possibilities for strain in the barrier layers **15:** unstrained, or compressively strained barriers. Usually, we prefer strain that is equal, but opposite sign, in the wells and barriers. This is called symmetric strain for the quantum stack. In that case, the **buffer layer upon which the MQW stack is grown should have a zincblende lattice parameter that is halfway between the lattice constant of the wells and the lattice constant of the barriers.** Symmetric strain allows a thick high-quality stack to be grown. The thickness of individual layers is chosen to be less than the critical layer thickness for stable strain, which gives monocrystal layers with very few misfit dislocations per cm. sq.*

We choose to call the MQW stack pseudomorphic" because all layers are coherently strained with near-perfect crystal quality (low defect density).

The in-plane lattice size of the wells and barriers conforms to the lattice size of the buffer. Thus, the buffer's lattice size is "reproduced" throughout the stack. *This is called commensurate growth or coherent strain. Strain is produced in the epitaxial layers by the mismatch between the buffer lattice parameter and the well-or-barrier lattice that would of existed in a bulk alloy crystal. The bulk lattice size is determined by the Ge/Sn ratio (the alloy composition).*

While Soref does discuss matching the "lattice size" of the buffer layer (layer #19, Figure 2) to the MQW stack layers and the strain produced in each as a result, the buffer layer described in Soref is not the presently claimed $Ge_{1-x-y}Si_xSn_y$ alloy. Accordingly, Soref does not explicitly or inherently anticipate an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer which is lattice matched to a second layer nor the use of same layer lattice matched essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer in the presently claimed structure.

For the preceding reasons, Applicants submit the rejection of each of the instant dependent claims over 35 USC 102(b) is improper. Applicants respectfully request reconsideration and withdrawal of each of the rejections.

B.   Rejection of Claims 3, 13, and 18 under 35 USC §102(b)

Claims 3, 13, and 18 stand rejected for allegedly being anticipated by Fieselmann, U.S. 4,777,023 ("Fieselmann"). Applicants respectfully disagree with the rejections.

1. Independent Claim 3

For a claim to be anticipated by the prior art, under 35 USC 102, the reference must recite all limitations of the allegedly anticipated claim. "A claim is anticipated only if each and every element as set forth in the claim is found, either expressly or inherently described, in a single prior art reference." *Verdegaal Bros. v. Union Oil Co. of California*, 814 F.2d 628, 631, 2 USPQ2d 1051, 1053 (Fed. Cir. 1987) MPEP 2131.

The Office has alleged that Fieselmann anticipates the compound, $H_3SiO_3SCF_3$, through the recitation at Column 2, Lines 37 - 46 (emphasis added),

To achieve the objects, and in accordance with the purpose of the invention, as embodied and broadly described herein, the invention comprises a

*method for preparing a hydride containing at least two different Group 4A atoms wherein at least one of the Group 4A atoms is silicon or germanium, comprising the steps of: (a) reacting an alkali metal and a macrocyclic compound with a silicon or germanium hydride to form a salt; and (b) reacting the salt formed in step (a) **with a halide** containing a different Group 4A atom.*

Claim 3 presently reads,

> 3. (Original) A method for synthesizing a compound having the molecular formula $H_3Si\text{-}GeH_3$, the method comprising combining $H_3SiO_3SCF_3$ with $KGeH_3$ under conditions whereby $H_3Si\text{-}GeH_3$ is obtained.

"A halide" is not explicitly defined in Fieselmann, rather examples of halides are provided, see Column 5, Line 35 – 39 (emphasis added),

> A wide variety of halides containing a different Group 4A atom can be used in practicing step (b) of the present invention. Good results have been obtained using CH_3I, CH_2Cl_2, or SiH_3Cl as the halide containing a different Group 4A atom.

Additionally, synthetic examples using "halides" are provided in Fieselmann which use the same starting materials which are exemplified in the preceding definition: Example 2, $SiH_3\underline{Cl}$; Example 3, $CH_3\underline{I}$; Example 4, $CH_2\underline{Cl}_2$; Example 5, $CH_2\underline{Cl}_2$.

The Office appears to believe that the presently claimed species [$H_3Si\text{-}OS(O)_2CF_3$] is a "halide" as defined in Fieselmann, and stated in the paragraph bridging pages 7 and 8 of the Final action in response to Applicant's previous arguments (bold emphasis added),

> However Applicants' position can be persuasive because If Soren [sic] reference meant only a halide and should be limited to halogens only (Flouride, chloride, bromide or iodide) then it was not necessary for Soren to mention **a compound containing a halide** component in a different 4a group atom ([underlined] emphasis supplied).

In the preceding quote, the Applicants presume that the Office means "a Group 4a compound containing a halide." The Office did not supply a citation to Fieselmann to support the alleged description.

However, Applicants submit that the presently claimed species ($H_3SiO_3SCF_3$) is not a "halide" as defined in Fieselmann. First, Fieselmann does not define either "a compound containing a halide," or "a halide containing.." or "the halide containing..."; rather Fieselmann defines "the halide containing a different Group 4A atom" by way of examples, at Col. 5, lines

35 – 39 (*supra*). Therefore, to properly define the term "halide" one must look at the "plain meaning" to one skilled in the art **unless such meaning is inconsistent with the specification.** **MPEP 2111.01 (emphasis added).**
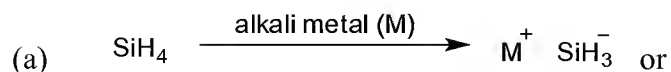
"Plain meaning" refers to the ordinary and customary meaning given to the term by those of ordinary skill in the art. The ordinary and customary meaning of a term may be evidenced by a variety of sources, including the words of the claims themselves, the remainder of the specification, the prosecution history, and extrinsic evidence concerning relevant scientific principles, the meaning of technical terms, and the state of the art. "Where there are several common meanings for a claim term, the patent disclosure serves to point away from the improper meanings and toward the proper meanings." *Renishaw PLC v. Marposs Societa' per Azioni*, 158 F.3d 1243, 1250, 48 USPQ2d 1117, 1122 (Fed. Cir. 1998). If more than one extrinsic definition is consistent with the use of the words in the intrinsic record, the claim terms may be construed to encompass all consistent meanings. See e.g., *Rexnord Corp. v. Laitram Corp.*, 274 F.3d 1336, 1342, 60 USPQ2d 1851, 1854 (Fed. Cir. 2001). "[W]ords in patent claims are given their ordinary meaning in the usage of the field of the invention, unless the text of the patent makes clear that a word was used with a special meaning. *Toro Co. v. White Consol. Indus., Inc.*, 199 F.3d 1295, 1299, 53 USPQ2d 1065, 1067 (Fed. Cir. 1999) **MPEP 2111.01(II).** The meaning of a particular claim term may be defined by implication, that is, according to the usage of the term in the context in the specification. See *Phillips v. AWH Corp.*, 415 F.3d 1303, 75 USPQ2d 1321 (Fed. Cir. 2005) (*en banc*); and *Vitronics Corp. v. Conceptronic Inc.*, 90 F.3d 1576, 1583, 39 USPQ2d 1573, 1577 (Fed. Cir. 1996). **MPEP 2111.01(III).**

To understand the definition of "halide" in Fieselmann, one must look to the examples therein. Fieselmann teaches methods for preparing "a hydride containing at least two different Group 4A atoms wherein at least one of the Group 4A atoms is silicon or germanium," comprising reacting

(a) the alkali salt of a silicon or germanium hydride; with

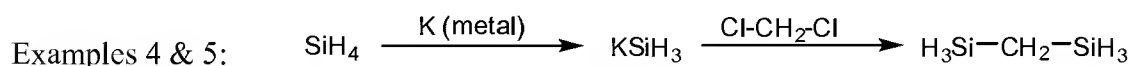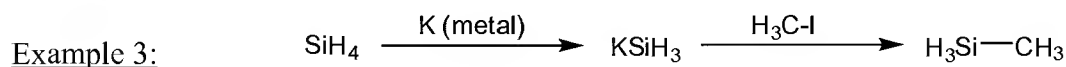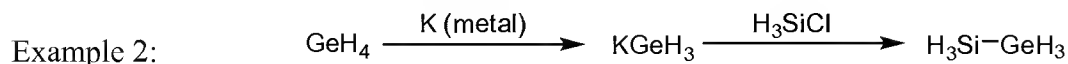(b) a halide containing a different Group 4A atom (see, Column 2, lines 36 – 46).

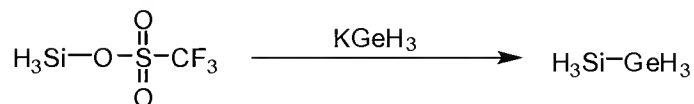That is, generically, Fleischmann describes the following:

$$(a) \quad SiH_4 \xrightarrow{\text{alkali metal (M)}} M^+ \ SiH_3^- \quad \text{or}$$

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$$GeH_4 \xrightarrow{\text{alkali metal (M)}} M^+ \; Ge\bar{H}_3$$

(b) For example, $M^+ \; Ge\bar{H}_3 \xrightarrow{\text{X-M'}} M'^-GeH_3$, where M' is a group IVa atom, but not Ge.

Fieselmann teaches the following specific examples:

Example 2: $GeH_4 \xrightarrow{\text{K (metal)}} KGeH_3 \xrightarrow{H_3SiCl} H_3Si{-}GeH_3$

Example 3: $SiH_4 \xrightarrow{\text{K (metal)}} KSiH_3 \xrightarrow{H_3C\text{-}I} H_3Si{-}CH_3$

Examples 4 & 5: $SiH_4 \xrightarrow{\text{K (metal)}} KSiH_3 \xrightarrow{Cl\text{-}CH_2\text{-}Cl} H_3Si{-}CH_2{-}SiH_3$

Applicants submit that "the halide" in Fieselmann is not any "compound containing a halide" as alleged by the office (*supra*). In each example described in Fieselmann, the halide is bound to the "Group 4A atom" to which the silyl or germyl group is subsequently bound by the reaction.   That is, "the halide" is acting as a "leaving group" in the reaction.   Such a definition is consistent with the exemplified "halides" at Col. 5, lines 35 – 39, and Example 2 – 5. Therefore, the term "halides" in Fieselmann, to one skilled in the art, merely means compounds containing a halogen atom where the halogen atom *itself* is (a) displaced by the nucleophile; **and** (b) bonded to the Group 4a atom which forms the new chemical bond to the silyl or germyl nucleophile.

In contrast, the instantly rejected claims generally describe the following reaction,

$$H_3Si{-}O{-}\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}{-}CF_3 \xrightarrow{KGeH_3} H_3Si{-}GeH_3$$

Applicants note that the germyl anion displaces the trifluoromethylsulfonyloxy (-OS(O)$_2$CF$_3$; triflate) group.   All halogen atoms in the triflate group are bound to a carbon atom which is merely part of the triflate group.   As is clear from the instant specification, the reaction occurs **at the silicon atom** and **not the carbon atom.**

Applicants submit that, while the $H_3SiO_3SCF_3$ in Claim 3 **contains** fluoro groups, the compound does not fall under the definition of the term "halide" as used in Fieselmann, and as would be understood by one skilled in the art for the following reasons,

(i) the fluoro groups of the instant triflate group are not **themselves,** displaced by germyl anion; rather **the entire triflate group (-OS(O)₂CF₃)** is displaced; and

(ii) the newly formed chemical bond in the claimed reaction is formed between the germyl group and the Si atom, not the carbon atom to which the fluoro groups are attached.

For the preceding reasons, the term "halide" in Fieselmann does not anticipate the instant starting material, H_3Si-$OS(O)_2CF_3$, nor does Fieselmann anticipate the claimed reaction using H_3Si-$OS(O)_2CF_3$. Applicants submit the rejection of the instant claims over 35 USC §102(b) is improper. Applicants respectfully request reconsideration and withdrawal of the rejection.

2. Dependent claims

a. Dependent claim 13

The Office has alleged that claim 13 is anticipated by Fieselmann, and cited the Examples therein. Claim 13 is dependent method claim of Claim 9, and is directed to a method to prepare a semiconductor structure comprising: a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer, further comprising the step of annealing the Sn_zGe_{1-z} layer prior to depositing the $Ge_{1-x-y}Si_xSn_y$ layer.

Fieselmann does not discuss depositing a $Ge_{1-x-y}Si_xSn_y$ layer over a Sn_zGe_{1-z} layer (Claim 9), nor does Fieselmann discuss annealing the Sn_zGe_{1-z} before depositing the $Ge_{1xy}Si_xSn_y$ layer (Claim 13). The discussion in Fieselmann regarding preparing a semiconductor structure is Example 7 which is concerned with the proposed preparation of a SiGe layer as an "i-layer" in a p-i-n junction (Col. 8, lines 59 – 64, referencing Figure 1). Applicants submit the rejection of claim 13 under 35 USC §102(b) is improper for failing to anticipate all the claimed limitations.

b. Dependent claim 18

The Office has alleged that claim 18 is anticipated by Fieselmann, and cited Example 3 therein. Claim 18 is dependent method claim of Claim 3, and is directed to a method for synthesizing a compound having the molecular formula $H_3Si\text{-}GeH_3$, with the further limitation that the reaction occurs at about -60 °C . Applicants note that Example 2 in Fieselmann is concerned with the preparation of $H_3Si\text{-}GeH_3$. Example 3 is concerned with the preparation of $H_3Si\text{-}\underline{C}H_3$.

Fieselmann does not describe methods for preparing $H_3Si\text{-}\underline{Ge}H_3$ where the reaction occurs at about -60 °C, as claimed. Preferred temperatures for the reaction in Fieselmann are described at Col. 5, lines 50 – 62, a range from -100 °C to 0 °C. The examples in Fieselmann use specific methods where reactants are mixed at

(a) liquid nitrogen temperatures (77 K; -196 °C) and warmed to room temperature (~ 25 °C) [Examples 2, 4, and 5]; or

(b) -38 °C [Example 3].

Applicants submit the rejection of claim 18 under 35 USC §102(b) is improper for failing to anticipate all the claimed limitations. For the preceding reasons, Applicants submit the rejections of claims 3, 13, and 18 under 35 USC §102(b) are improper. Applicants respectfully request reconsideration and withdrawal of the rejection.

C.   Rejection of Claims 9 - 17 under 35 USC §112, 2nd paragraph

In the present Final Office Action, Claims 9 – 17 are rejected for allegedly being indefinite. The Office has stated that *"It is unclear whether claims 9 to 17 are claiming a method or a product. Claims 9 10 17 recite 'a method as {ultimately} claimed in claim 1..' but claim 1 is a product claim rendering claims 9 to 17 indefinite."* Applicants respectfully traverse.

Claim 9 presently reads, (emphasis added)

*9. **A method to prepare** the semiconductor structure according to claim 1,*
comprising the steps of,

    providing a substrate;

    depositing a Sn_zGe_{1-z} layer over the substrate; and

    depositing a $Ge_{1-x-y}Si_xSn_y$ layer over the Sn_zGe_{1-z} layer.

As the preamble states, claim 9 is clearly a method claim. Reference to Claim 1 is merely present to define the scope of the claim, and in particular, the nature of the $Ge_{1-x-y}Si_xSn_y$ layer. According to MPEP 2173.05(f) (emphasis added),

> *A claim which makes reference to a preceding claim to define a limitation is an acceptable claim construction which should not necessarily be rejected as improper or confusing under 35 U.S.C. 112, second paragraph. [...] See also Ex parte Porter, 25 USPQ2d 1144 (Bd. Pat. App. & Inter. 1992) where reference to "the nozzle of claim 7" in a method claim was held to comply with 35 U.S.C. 112, second paragraph. However, where the format of making reference to limitations recited in another claim results in confusion, then a rejection would be proper under 35 U.S.C. 112, second paragraph.*

Applicants submit that the reference to claim 1 in presently rejected claim 9 does not create confusion in interpreting the claim and as such the rejection under 35 USC §112, 2nd paragraph is improper, and respectfully request reconsideration and withdrawal of the rejection.

D.   Conclusion

For the reasons set forth above, Soref and Fieselmann cannot support the present claim rejections. Further, Claim 9 is not indefinite as the metes and bounds of the claim are not ambiguous. Accordingly, the applicants respectfully submit that the present rejections are improper and should be withdrawn. Passage of the claims to issue is respectfully requested.

Respectfully submitted,

Date: December 6, 2007

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VIII.   CLAIMS APPENDIX

1. (Previously presented) A semiconductor structure comprising: a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and an essentially single-phase $Ge_{1-x-y}Si_xSn_y$ layer formed over the Sn_zGe_{1-z} layer.

2. (Original) The semiconductor structure of claim 1 wherein the substrate comprises silicon.

3. (Original) A method for synthesizing a compound having the molecular formula H_3Si-GeH_3, the method comprising combining $H_3SiO_3SCF_3$ with $KGeH_3$ under conditions whereby H_3Si-GeH_3 is obtained.

4. (Previously presented) The structure of claim 1, wherein z is about 0.01 to about 0.05.

5. (Previously presented) The structure of claim 1, wherein x is about 0.01 to about 0.25; and y is about 0.01 to about 0.11.

6. (Previously presented) The structure of claim 1, wherein x is about 0.01 to about 0.25; y is about 0.01 to about 0.11; z is about 0.01 to about 0.05; and the substrate comprises silicon.

7. (Previously presented) The structure of claim 1, wherein the $Ge_{1-x-y}Si_xSn_y$ layer is strained.

8. (Previously presented) The structure of claim 1, wherein the $Ge_{1-x-y}Si_xSn_y$ layer is relaxed.

9. (Previously presented) A method to prepare the semiconductor structure according to claim 1, comprising the steps of,

> providing a substrate;

> depositing a Sn_zGe_{1-z} layer over the substrate; and

> depositing a $Ge_{1-x-y}Si_xSn_y$ layer over the Sn_zGe_{1-z} layer.

10. (Previously presented) The method of claim 9, wherein the $Ge_{1-x-y}Si_xSn_y$ layer is deposited by precursor chemical vapor deposition, wherein the precursor chemical vapor comprises SnD_4 and H_3SiGeH_3.

11. (Previously presented) The method of claim 9, wherein the Sn_zGe_{1-z} layer is deposited by precursor chemical vapor deposition, wherein the precursor chemical vapor comprises SnD_4 and Ge_2H_6.

12. (Previously presented) The method of claim 9, wherein the substrate comprises silicon.

13. (Previously presented) The method of claim 9, further comprising the step of

annealing the Sn_zGe_{1-z} layer prior to depositing the $Ge_{1-x-y}Si_xSn_y$ layer.

14. (Previously presented) The method of claim 9, wherein z is about 0.01 to about 0.05.

15. (Previously presented) The method of claim 9, wherein x is about 0.01 to about 0.25; and y is about 0.01 to about 0.11.

16. (Previously presented) The method of claim 9, wherein x is about 0.01 to about 0.25; y is about 0.01 to about 0.11; z is about 0.01 to about 0.05; and the substrate comprises silicon.

17. (Previously presented) The method of claim 9, wherein the $Ge_{1-x-y}Si_xSn_y$ layer is deposited at a temperature of about 310°C to about 375°C.

18. (Previously presented) The method of claim 3, wherein the $H_3SiO_3SCF_3$ and $KGeH_3$ are combined at about -60°C.

19. (Previously presented) An alloy of the formula, $Ge_{1-x-y}Si_xSn_y$, wherein x is about 0.01 to about 0.25 and y is about 0.01 to about 0.11.

20. (Previously presented) The alloy of Claim 19, wherein x is about 0.13 to about 0.20.

21. (Previously presented) The alloy of Claim 20, wherein y is about 0.07 to about 0.11.

22. (Previously presented) The alloy of Claim 20, wherein y is about 0.01 to about 0.06.

23. (Previously presented) A semiconductor structure comprising: a substrate, a Sn_zGe_{1-z} layer formed over the substrate, and a layer of the alloy of Claim 19 formed over the Sn_zGe_{1-z} layer.

24. (Previously presented) The semiconductor structure of claim 23 wherein the substrate comprises silicon.

25. (Previously presented) The semiconductor structure of Claim 1 wherein the Sn_zGe_{1-z} and $Ge_{1-x-y}Si_xSn_y$ layers are lattice-matched.

26. (Previously presented) The semiconductor structure of Claim 23 wherein the Sn_zGe_{1-z} and $Ge_{1-x-y}Si_xSn_y$ layers are lattice-matched.

27. (Previously presented) A structure comprising: a Sn_zGe_{1-z} layer and a layer of the alloy of Claim 19 formed over the Sn_zGe_{1-z} layer.

IX.   EVIDENCE APPENDIX

Aella, et al. Appl. Phys. Lett. 2004, 84, 888 ('Aella')

Optical and structural properties of $Si_xSn_yGe_{1-x-y}$ alloys

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Single-phase $Si_xSn_yGe_{1-x-y}$ alloys ($x \leq 0.25, y \leq 0.11$) were grown on Si using chemical vapor deposition. First principles simulations predict that these materials are thermodynamically accessible and yield lattice constants as a function of Si/Sn concentrations in good agreement with experiment. An empirical model derived from experimental Si_xGe_{1-x} and Sn_yGe_{1-y} binary data also provides a quantitative description of the composition dependence of the lattice parameters. Spectroscopic ellipsometry of selected samples yields dielectric functions indicating a band structure consistent with highly crystalline semiconductor materials of diamond symmetry. Incorporation of Si into Sn_yGe_{1-y} leads to an additional reduction of the E_2 critical point, as expected based on the E_2 values of Si and Ge. © *2004 American Institute of Physics.*
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The great success of III–V quaternary semiconductors for independent band-gap and strain engineering has led to widespread applications.[1] For Si-based materials, the Si–Sn–Ge ternary system should have a similar impact in the group IV arena. The intriguing potential of random SiSnGe alloys has recently been discussed by Soref and Perry,[2] and its band structure for Si-rich concentrations has been explored by Johnson and Ashcroft.[3] Our own preliminary study describes the first successful growth of this material.[4] Nevertheless, experimentally these alloys remain virtually unexplored. In this article, we report development and rational design of device-quality concentrations, which are suitable for optical investigations as well as *ab initio* simulation. These materials possess a variable *and* controllable range of compositions, and exhibit lattice constants above and below that of bulk Ge thus providing unique opportunities for band-gap and strain engineering in group IV alloys. Possible applications, aside from those highlighted by Soref and Perry,[2] include buffer layers for the growth of relaxed SiGe alloys with high Ge content, and barrier layers for novel type-I direct gap Ge quantum wells.

Our target compositions were derived from the well known Sn_xGe_{1-x} ($x = 2 - 10\%$) alloys by substituting Ge in the Sn–Ge lattice by Si. The present growth studies immediately produced a range of stable alloys including those with compositions $Si_{0.18}Sn_{0.10}Ge_{0.72}$, $Si_{0.20}Sn_{0.08}Ge_{0.72}$, $Si_{0.18}Sn_{0.065}Ge_{0.755}$, $Si_{0.13}Sn_{0.06}Ge_{0.81}$, $Si_{0.13}Sn_{0.03}Ge_{0.84}$, and $Si_{0.20}Sn_{0.02}Ge_{0.78}$. These compositions are particularly attractive since they are readily amenable to first principles simulations using a standard 64-atom supercell representation $Si_{12}Sn_6Ge_{46}$, $Si_{13}Sn_5Ge_{46}$, $Si_{12}Sn_4Ge_{48}$, $Si_8Sn_4Ge_{52}$, $Si_8Sn_2Ge_{54}$, and $Si_{13}Sn_1Ge_{50}$. Table I shows the close correspondence between the model concentrations and those of the synthesized alloys. A structural model of the high Sn

content alloy $Ge_{46}Si_{13}Sn_5$ (20.3% Si, 71.9% Ge, 7.8% Sn) is shown in Fig. 1.

All $Si_xSn_yGe_{1-x-y}$ alloys were grown *in situ* on Si(100) by reacting appropriate concentrations of SiH_3GeH_3 with SnD_4 between 310–370 °C on lattice matched Sn_xGe_{1-x} ($x = 2 - 4$ at. %) buffer layers. The substrates were prepared using a modified (RCA) process followed by hydrogen surface passivation and the growth was conducted in the presence of large concentrations of research grade H_2 at 10^{-2} Torr (typical base pressure was 1×10^{-9} Torr). The samples were then grown by systematically adjusting the temperature, pressure, and reactant concentrations. In all cases device quality materials with single-phase concentrations and random diamond cubic structures were obtained. Rutherford backscattering (RBS) analysis revealed a two-layer heterostructure with thickness of 70–100 nm for the $Si_{1-x-y}Ge_xSn_y$ films and 50–100 nm for the Sn_xGe_{1-x} buffer layers. The range of atomic concentrations as measured by RBS were 13–20 % Si, 62–85 % Ge, and 1–11 % Sn (see Table I for selected samples). The maximum Sn content samples (11–7 % Sn) were deposited reproducibly between 310 and 340 °C, respectively, while at higher temperatures (350–375 °C) the deposition yielded lower Sn concentrations of 6–1 at. %.

Figure 2(a) compares random and aligned RBS spectra for a representative $Si_{0.20}Sn_{0.08}Ge_{0.72}$ alloy grown on a $Sn_{0.02}Ge_{0.98}$ buffer layer. The high degree of He ion channeling found for Si, Ge, and Sn confirms full substitutionality of the elements in the structure, and indicates the formation of epitaxial materials. This was also confirmed by high resolution cross sectional electron microscopy (XTEM), atomic force microscopy (AFM), and x-ray diffraction (rocking curves) which revealed highly aligned layers with monocrystalline structures and atomically smooth surfaces. This is demonstrated in Fig. 2(b) which shows a dark field image of the entire $Si_{0.20}Sn_{0.08}Ge_{0.72}/Sn_{0.02}Ge_{0.98}/Si$ heterostructure. In general we find that the crystallinity in these samples is far superior with respect to our preliminary work.[4] This is primarily due to an *in situ* annealing step of the buffer layer which results in an overall reduction of threading defects, particularly those terminating at the top surface. This pro-

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TABLE I. Comparison of "best estimates" based on *ab initio* calculations (see text for explanation) and experimental lattice constants for selected samples. Top panel: energy, free energy, and lattice constants obtained from first principles local density approximation calculations. Bottom panel: comparison of Vegard's law (VEG) and empirical formula results (LC) with experiment. Values in parentheses indicate percent deviation from experimental Ge lattice constant (5.658 Å).

%Si	%Ge	%Sn	ΔE (meV)	ΔG^{300} (meV)	a_{LDA}^{*} (Å)	%Si	%Ge	%Sn	a_{VEG} (Å)	a_{LC} (Å)	a_{EXP} (Å)
18.8	71.9	9.4	31.0	11.6	5.689 (+0.5)	18	72	10	5.700 (+0.7)	5.712 (+0.9)	5.684 (+0.5)
20.3	71.9	7.8	29.4	10.4	5.672 (+0.3)	20	72	8	5.679 (+0.4)	5.687 (+0.5)	5.668 (+0.2)
18.8	75.0	6.3	23.9	6.3	5.663 (+0.1)	18	75.5	6.5	5.671 (+0.2)	5.678 (+0.3)	5.680 (+0.4)
14.1	79.6	6.3	21.7	6.0	5.686 (+0.5)	14	80	6	5.676 (+0.3)	5.683 (+0.4)	5.690 (+0.6)
12.5	84.4	3.1	14.7	1.9	5.652 (−0.1)	13	84	3	5.654 (−0.1)	5.656 (0.0)	5.644 (−0.3)
20.3	78.1	1.6	13.9	−0.6	5.619 (−0.7)	20	78	2	5.629 (−0.5)	5.629 (−0.5)	5.630 (−0.5)

vides a highly ordered and defect free interface for subsequent growth of SiSnGe. Remarkably for all samples, the root mean square surface roughness, as measured by AFM, is 0.5 to 1.0 nm. A high-resolution micrograph of the $Si_{0.20}Sn_{0.08}Ge_{0.72}/Sn_{0.04}Ge_{0.96}$ interface [Fig. 2(d)] clearly shows a commensurate and virtually defect-free microstructure. Micrographs of the buffer layers show that the lattice mismatch between the two materials is accommodated by periodic edge dislocations located at the interface [see Fig. 2(c)]. These are parallel to the interface plane rather than parallel to the growth direction as in threading dislocations, which are known to degrade the crystallinity and the electrical properties of the film. Complementary x-ray diffraction studies confirm single-phase, strain free materials with an average diamond cubic structure. Rocking curves of the SiSnGe (004) reflection give full width at half maxima of 0.25–0.30°. The unit cell parameters obtained from the diffraction data are in close agreement with the theoretical values obtained from first principle simulations (see Table I below). The compositional homogeneity and the phase purity of the films were investigated by Auger electron spectroscopy (AES) and electrons energy loss spectroscopy. The AES data revealed highly homogeneous elemental profiles throughout each layer of the heterostructure and showed sharp changes of composition across each interface. Electron-energy-loss spectroscopy (EELS) profiles showed that the constituent elements appeared together at every nanometer region probed with no indication of phase segregation and Sn precipitation.

Next, we investigated the electronic band structures of $Si_xSn_yGe_{1-x-y}$ using spectroscopic ellipsometry. The pseudodielectric functions of such alloys (see Fig. 3) grown using Sn_yGe_{1-y} buffers on Si are not easy to fit, since this requires a four-layer model (substrate/Sn_yGe_{1-y} buffer/ $Si_xSn_yGe_{1-x-y}$/surface overlayer). We solve this problem using the dielectric functions for Sn_yGe_{1-y} determined previously,[5] which leaves only the optical constants of $Si_xSn_yGe_{1-x-y}$ and the thicknesses of the buffer, the ternary alloy, and the surface overlayer (oxide and/or roughness) as parameters. This procedure yields thicknesses comparable to those obtained by XTEM and reproducible dielectric functions for $Si_xSn_yGe_{1-x-y}$, especially at high photon energies near the E_2 critical point (see above) where the penetration depth of the light is smaller than the $Si_xSn_yGe_{1-x-y}$ film thickness. The dielectric function of $Si_xSn_yGe_{1-x-y}$ has a similar shape compared to that of Ge or Sn_yGe_{1-y}, indicating highly crystalline single-phase quality and semiconducting character as expected for an alloy with cubic crystal symmetry.[6,7] Using the same derivative technique as in Ref. 5, we determine the E_2 energies of several $Si_xSn_yGe_{1-x-y}$ samples from the dielectric function. The latter contain peaks related to interband transitions at different regions of the Brillouin zone.[6] For the experimental reasons mentioned
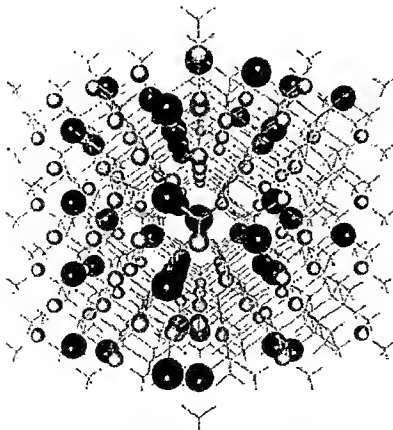

FIG. 1. Structure of the highly saturated $Si_{13}Sn_5Ge_{46}$ alloy (20.3% Si, 7.8% Sn, and 71.9% Ge) obtained from first-principles optimization of all cell dimensions and atomic positions. View is along the (110) direction. White and black spheres are Si and Sn, respectively, while the Ge lattice structure is shown using gray lines (atoms not shown for clarity). Note that in spite of the high density of Si/Sn constituents the free energy of formation is only slightly metastable (10.4 meV) for the random structure shown.
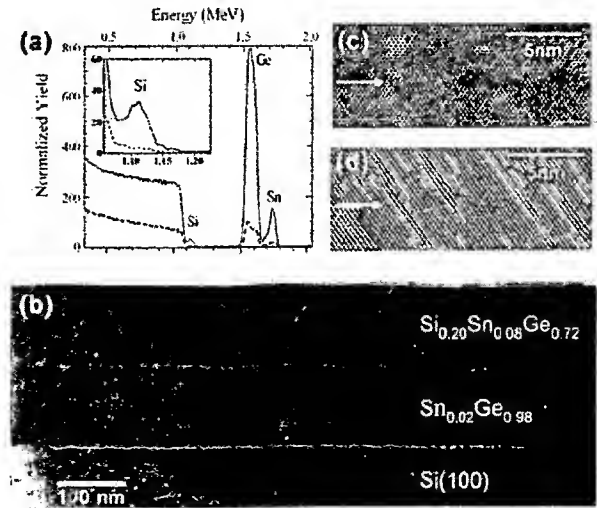

FIG. 2. (a) RBS aligned (solid line), and random (dotted line) spectra of $Si_{0.20}Sn_{0.08}Ge_{0.80}$ epilayer and $Sn_{0.04}Ge_{0.96}$ buffer layer showing a highly aligned heterostructure. Low and high intensity Sn peaks correspond to the buffer and epilayer, respectively. Inset: magnified view of the Si peak, (b) XTEM of the entire $Si_{0.20}Sn_{0.08}Ge_{0.72}/Sn_{0.02}Ge_{0.98}/Si(100)$ heterostructure, (c) $Si(100)/Sn_{0.02}Ge_{0.98}$ interface (indicated by arrow), and (d) $Si_{0.20}Sn_{0.08}Ge_{0.72}/Sn_{0.02}Ge_{0.98}$ interface.
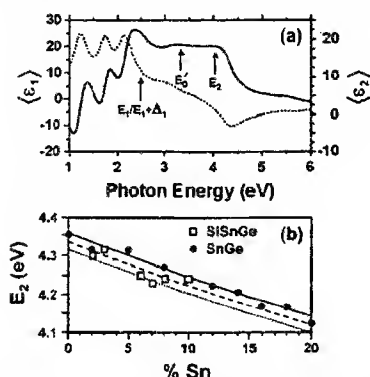
FIG. 3. (a) Pseudodielectric function of $Si_{0.20}Sn_{0.02}Ge_{0.78}$ (imaginary part-solid, real part-dashed) Interband critical points are indicated. (b) E_2 critical point energy for Sn_yGe_{1-y} (circles) from Ref. 5 with a single-parameter fit based on the E_2 energies of bulk Ge and Sn and a small negative bowing (solid line). The E_2 energies of $Si_xSn_yGe_{1-x-y}$ (squares) show an additional reduction due to incorporation of Si which can be estimated for 10 and 20% Si (dashed, dotted) from the dependence of E_2 in Si_xGe_{1-x} (see Ref. 7).

above, we focus on the E_2 critical point, related to transitions at and near the x-point from the highest valence band to the lowest conduction band. Both Sn and Si reduce E_2 compared to Ge (4.36 eV). The variation of E_2 in Sn_yGe_{1-y} was determined previously[5] (see Fig. 3). An additional reduction of E_2 is found when adding Si. All $Si_xSn_yGe_{1-x-y}$ samples (squares) display E_2 energies below those of Sn_yGe_{1-y} with the same Sn content (i.e., are located below the solid line). To estimate this additional reduction, we calculate E_2 of $Si_xSn_yGe_{1-x-y}$ from the values for Sn_yGe_{1-y} and Si_xGe_{1-x} determined earlier,[5,7] assuming the same quadratic bowing for E_2 in Si_xGe_{1-x} as for E_1. Within this framework, the E_2 energies for five different $Si_xSn_yGe_{1-x-y}$ alloys are as expected for 10 and 20% Si. Small deviations from this model can be explained by the uncertainty in the numerical procedure (10–20 meV for E_2) and small residual stresses between the ternary alloy and the binary Sn_yGe_{1-y} buffer, which will lead to strain shifts of the critical points.[7]

Experimentally we find that the ternary SiSnGe alloys form more readily, and exhibit greater thermal stability than their SnGe counterparts. This may be due to the strain equalization resulting from the opposing effects of the Si and Sn incorporation. These observations prompted us to explore the thermodynamic stability from a theoretical perspective. Accordingly the alloys were investigated using first principles simulations[8] in a 64-atom supercell representation, e.g., $Si_{13}Sn_5Ge_{46}$ (20.3% Si, 7.8% Sn, and 71.9% Ge) in which the Sn and Si atoms are randomly distributed on a Ge lattice (see Table I). Shape and volume optimization was carried out while fully relaxing all internal atomic coordinates to an accuracy of 0.001 eV/Å (ultrasoft pseudopotentials were used with $E_{cut} \sim 350$ eV and 14 irreducible k-points). Elemental Si, Ge, and Sn calculated using the same procedure yielded the expected perfect diamond lattice symmetry with $a_{Si} = 5.3894$ Å, $a_{Ge} = 5.6251$ Å, and $a_{Sn} = 6.4546$ Å, respectively, in good agreement with experimental values ($a_{Si} = 5.431$ Å, $a_{Ge} = 5.658$ Å, and $a_{Sn} = 6.493$ Å). Table I lists the calculated alloy lattice constants obtained by averaging the three super cell edge lengths (variance <0.004 Å) and the static lattice alloy formation energies $\Delta E = E[Si_xSn_yGe_z] - x\ E[Si] - y\ E[Sn] - z\ E[Ge]$, where $z = 1 - x - y$. The Gibbs free energy at ambient pressure was

approximated   as $\Delta G(T;x,y) \sim \Delta E(x,y) - T\Delta S_{mix}(x,y)$ where the last term represents the ideal entropy of mixing. Our results indicate that the low %Sn alloys are thermodynamically stable while the 7–8% Sn alloys are only slightly metastable (*n.b.*, k_BT at 300° $\sim$25 meV). The local bonding around Si and Sn sites deviates from ideal (diamond) behavior indicating a significant degree of internal lattice relaxation even though the cell volume remains close to a Vegard law value. The values a_{LDA}^* (Table I) were obtained by scaling the alloy local density approximation lattice constants such that those calculated for Si, Ge, and Sn match experiment. The resulting values agree with experiment to within $\sim$0.01 Å or 0.2% and generally track the variations in composition observed experimentally.

This behavior can also be estimated from available data for the Si_xGe_{1-x} and Sn_yGe_{1-y} binary systems. For Si_xGe_{1-x} the lattice constant is known[9] to behave as $a_{SiGe}(x) = a_{Si}x + a_{Ge}(1-x) + \theta_{SiGe}x(1-x)$ with $\theta_{SiGe} = -0.026$ Å, while a best fit to recent data[10] for Sn_yGe_{1-y} (for %Sn <20%) yields $a_{SnGe}(y) = a_{Sn}y + a_{Ge}(1-y) + \theta_{SnGe}y(1-y)$ with $\theta_{SnGe} = +0.166$ Å. These coefficients can then be combined to yield the formula (LC in Table I) $a_{SiSnGe}(x,y) = a_{Ge} + \Delta_{SiGe}x + \theta_{SiGe}x(1-x) + \Delta_{SnGe}y + \theta_{SnGe}y(1-y)$ where $\Delta_{SiGe} = a_{Si} - a_{Ge}$ and $\Delta_{SnGe} = a_{Sn} - a_{Ge}$. The role of the cross term (neglected here) involving the Si–Sn concentration product will form the subject of a subsequent paper.

A range of device quality $Si_xSn_yGe_{1-x-y}$ alloys with unprecedented Sn content have been grown and characterized. Spectroscopic ellipsometry analysis of these materials yields dielectric functions as expected for a crystalline alloy with cubic symmetry. Incorporation of Si into SnGe yields an additional reduction of the E_2 critical point, as expected based on the E_2 values of Si and Ge. The structure-composition relationship observed agrees well with first principles simulations and exhibits small deviations from Vegard's law behavior.

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Synthesis of ternary SiGeSn semiconductors on Si(100) via Sn$_x$Ge$_{1-x}$ buffer layers

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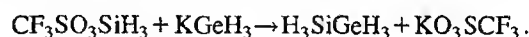
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Single-phase Si$_{1-x-y}$Ge$_x$Sn$_y$ alloys with random diamond cubic structures are created on Si(100) via ultrahigh vacuum chemical vapor deposition reactions of SnD$_4$ with SiH$_3$GeH$_3$ at 350 °C. Commensurate heteroepitaxy is facilitated by Ge$_{1-x}$Sn$_x$ buffer layers, which act as templates that can conform structurally and absorb the differential strain imposed by the more rigid Si and Si–Ge–Sn materials. The crystal structure, elemental distribution and morphological properties of the Si$_{1-x-y}$Ge$_x$Sn$_y$/Ge$_{1-x}$Sn$_x$ heterostructures are characterized by high-resolution electron microscopy, including electron energy loss nanospectroscopy, x-ray diffraction (rocking curves) and atomic force microscopy. These techniques demonstrate growth of perfectly epitaxial, uniform and highly aligned layers with atomically smooth surfaces and monocrystalline structures that have lattice constants close to that of Ge. Rutherford backscattering ion channeling shows that the constituent elements occupy random substitutional sites in the same average diamond cubic lattice and the Raman shifts are consistent with the lattice expansion produced by the Sn incorporation into SiGe tetrahedral sites. © 2003 American Institute of Physics. [DOI: 10.1063/1.1606104]

Metastable Ge$_{1-x}$Sn$_x$ alloys analogous to the well-known Si$_{1-x}$Ge$_x$ system have attracted considerable attention because of predictions that these materials might possess technologically important properties such as superior electron mobilities and tunable band gaps in the midinfrared.[1,2] More importantly, the band gap is expected to undergo an indirect-to-direct transition at compositions near $x=0.20$. Accordingly, considerable efforts have been devoted to growing Ge-rich Ge$_{1-x}$Sn$_x$ alloys on Ge substrates and buffer layers via molecular beam epitaxy (MBE).[3–5] Recently, we demonstrated, the growth of strain-free, device-quality Ge$_{1-x}$Sn$_x$ films directly on Si substrates using ultrahigh vacuum chemical vapor deposition (UHV-CVD).[6] The growth proceeds at low temperatures, between 250 and 350 °C, which makes it possible to grow thick films (50–500 nm) with extremely low defect densities and Sn concentrations up to 20%. The films are of such high quality that individual optical transitions can be readily identified and compared with those of Ge.[7] In particular, we find a dramatic reduction of the direct band gap E_0, which shrinks from 0.805 eV in Ge to 0.41 eV in Sn$_{0.14}$Ge$_{0.86}$.

The successful formation of Ge$_{1-x}$Sn$_x$ has prompted us to undertake research aimed at synthesis of the virtually unexplored Si–Ge–Sn ternary analog. Since the lattice parameter of Ge (5.657 Å) is intermediate between that of Si (5.43 Å) and of α-Sn (6.49 Å), Si$_{1-x-y}$Ge$_x$Sn$_y$ materials containing a suitable level of Sn could lattice match Ge, thereby allowing epitaxial growth of Ge/Sn$_x$Ge$_{1-x}$ heterostructures and related photonic devices based solely on group IV materials.[8] Moreover, this ternary system offers the potential of band gap engineering and tuning of the optical properties.[9]

We have recently computed the properties of strained Ge grown on relaxed Si$_{1-x-y}$Ge$_x$Sn$_y$ and we find that for appropriately selected Si/Sn ratios the heterostructure is a direct gap type I system with both electrons and holes confined in the pure Ge layers. This remarkable prediction warrants an intensive program to develop Si–Ge–Sn alloys.

Our synthetic strategy for preparation of Si–Ge–Sn is focused on UHV-CVD reactions of the gaseous compound SiH$_3$GeH$_3$ with SnD$_4$. The former is a derivative of GeH$_3$GeH$_3$ in which one of the GeH$_3$ groups is replaced with SiH$_3$ thus forming a molecular core with direct Si–Ge bonds. H$_3$SiGeH$_3$ is synthesized via a high yield method outlined below.

$$CF_3SO_3SiH_3 + KGeH_3 \rightarrow H_3SiGeH_3 + KO_3SCF_3.$$

Prior to growing Si–Ge–Sn we performed controlled experiments that involved the thermal dehydrogenation of H$_3$SiGeH$_3$ to study the deposition characteristics of this compound on Si(100) and thereby determine optimum conditions for growth of the target Si–Ge–Sn concentrations. We found that complete decomposition of H$_3$SiGeH$_3$ occurs at 450–700 °C and yields coherent SiGe quantum dots. Only partial decomposition takes place between 450 and 375 °C and forms amorphous films and no significant decomposition was obtained at 350 °C indicating that this temperature might be a reasonable starting point at which to initiate reactions of SiH$_3$GeH$_3$ and SnD$_4$ and produce Si–Ge–Sn films. Our previous studies have also indicated that 350 °C is the optimum temperature for incorporation of 2–6 at. % Sn into Ge lattice sites without any segregation and Sn precipitation.

The growth of Si$_{1-x-y}$Ge$_x$Sn$_y$ was initially investigated directly on Si(100). The reactions of H$_3$SiGeH$_3$ and SnD$_4$ at 350 °C produced thick layers of hydrogenated Si$_{1-x-y}$Ge$_x$Sn$_y$ films, indicating that the presence of Sn increases the reactivity of the precursor and facilitates film growth via facile elimination of H$_2$ from the Si–H and

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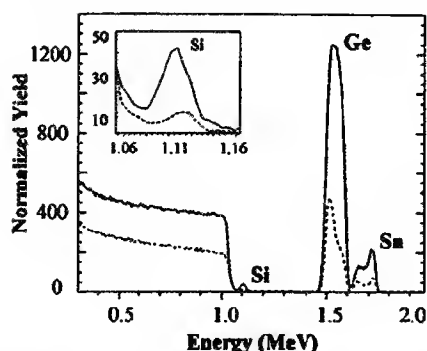[d]Electronic mail: jkouvetakis@asu.edu

FIG. 1. RBS random and channeled (dotted line) spectra of a $Si_{0.14}Ge_{0.80}Sn_{0.06}$ epilayer and a $Ge_{0.96}Sn_{0.04}$ buffer layer. Inset shows enlarged view of Si peak which channels remarkably well indicating complete substitutionality of Si atoms in the lattice.

FIG. 2. X-ray pattern ($\theta-2\theta$ scan) for the $Si_{0.14}Ge_{0.84}Sn_{0.02}/Ge_{0.97}Sn_{0.03}$ heterostructure. The higher intensity peak with $a=5.696$ Å is the (004) reflection of the buffer layer. The peak with $a=5.644$ Å is (004) reflection of the $Si_{0.14}Ge_{0.84}Sn_{0.02}$ overlayer. The line shows the location of the corresponding peak of pure Ge for comparison.

Ge–H bonds. Since the films grown in this fashion were amorphous, we explored next the use of buffer layers of $Ge_{1-x}Sn_x$ ($x=3-4$ at. %) to induce epitaxial film formation. We chose $Ge_{1-x}Sn_x$ alloys because they grow as highly uniform, strain-free layers with smooth surface morphologies and display extremely low concentrations of threading defects. In addition, they are high compressibility (softer) solids compared to either Si and $Si_{1-x-y}Ge_xSn_y$ and thereby can conform structurally and readily absorb the strain imposed by the more rigid Si and Si–Ge–Sn.

The $Ge_{1-x}Sn_x$ buffer layers were grown on Si(100) via reactions of Ge_2H_6 and SnD_4 at 350 °C. The growth of the $Si_{1-x}Ge_xSn_y$ films was conducted immediately thereafter, *in situ*, via reactions of appropriate concentrations of SnD_4 and H_3SiGeH_3. Rutherford backscattering (RBS) was used to determine the bulk composition and to estimate the film thickness. RBS channeling was used to determine the quality of the epitaxial growth and the degree of substitutionality of the elements in the structure. The RBS analyses showed that films with compositions ranging from $Si_{0.14}Ge_{0.84}Sn_{0.02}$ to $Si_{0.14}Ge_{0.80}Sn_{0.06}$ were grown on $Ge_{1-x}Sn_x$. The Sn content was readily increased from 2 to 6 at. % in controlled fashion by adjusting the partial pressure of SnD_4 in the reaction mixture. The Si incorporation remained constant, about 14 at. %, for all depositions conducted at 350 °C and was independent of the Sn concentration. The RBS aligned spectra showed that Si, Ge and Sn channeled remarkably well. The ratio between the aligned and random peak heights, which measures the degree of channeling of the He ions, was identical for all elements in a given sample. This indicates that Si, Ge and Sn occupy substitutional sites in the same diamond cubic structure and that the film is commensurate with the Si substrate. Figure 1 shows the RBS random and aligned spectra for the $Si_{0.14}Ge_{0.80}Sn_{0.06}/Ge_{0.96}Sn_{0.04}/Si$ heterostructure. Note that the Sn signal of the entire layer consists of two peaks, a narrow high energy peak corresponding to the epilayer, and the adjoining low energy Sn peak of the buffer layer. The Sn concentrations in each layer are 6 and 4 at. %, respectively. The epilayer and buffer layer thickness (determined from the peak width) are 45 and 115 nm, respectively (the RBS derived thickness is within 2% of the values obtained by cross-sectional electron microscopy). The small peak located next to the Si substrate signal is due to Si in the epilayer. The Si peak is well separated from the substrate signal indicating the absence of Si in the buffer layer.
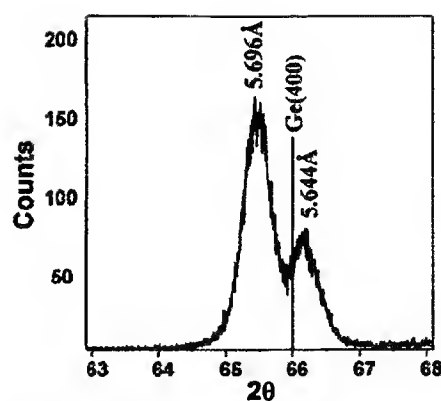
The film structure was investigated by x-ray diffraction and high-resolution cross-sectional electron microscopy (XTEM). The x-ray data revealed single-phase crystalline films, with no evidence of $Si_{1-x}Ge_x$, Si or Ge segregation. The cell parameter, a, obtained from the (004) reflection for samples with 6 at. % Sn was 5.694 Å which is nearly identical to that of the $Ge_{0.96}Sn_{0.04}$ buffer layer (5.70 Å). The 5.694 Å value is close to that predicted by Vegard's law, which in this case assumes linear interpolation between the lattice constants of Si and $Ge_{1-x}Sn_x$ where x is the Sn content in the sample. Figure 2 shows the x-ray spectrum of $Si_{0.14}Ge_{0.84}Sn_{0.02}$ grown via a $Ge_{0.97}Sn_{0.03}$ buffer layer. The (004) reflections give lattice parameters of 5.644 Å for the $Si_{0.14}Ge_{0.84}Sn_{0.02}$ layer and 5.696 Å for the buffer layer. The 5.644 Å value is close to that of Ge (5.657 Å) indicating that we have synthesized a ternary alloy that nearly lattice matches Ge. Rocking scans of the (004) reflections gave full width at half maxima between 0.25° and 0.50°, indicating a tightly aligned crystal mosaics.

The XTEM studies revealed thick single crystal films with low concentrations of threading defects. Electron micrographs that demonstrate high quality growth of a $Si_{0.14}Ge_{0.84}Sn_{0.02}$ sample on a $Ge_{0.97}Sn_{0.03}$ buffer layer are shown in Fig. 3. A typical image of the $Si(100)/Ge_{0.97}Sn_{0.03}$ interface region shows the presence of occasional twins and {111} stacking faults which seem to annihilate above the interface. The main defects that accommodate the large misfit between the two materials are Lomer edge dislocations, which are parallel to the interface plane. AFM shows a typical rms roughness of 0.6–1.5 nm. The XTEM images show that all layers are uniform in thickness and confirm smooth and continuous surface morphologies (Fig. 4). The elemental uniformity across the layer was investigated with energy dispersive x-ray (EDX) and electron energy loss (EELS) spectroscopies with nanometer sized probes. The nanospectroscopies showed a homogeneous distribution of Ge and Sn throughout the buffer layer, which is consistent with single-phase material. Analysis across the epilayer revealed significant concentrations of Si, Sn and a large concentration of Ge. The constituent elements appeared together at every nanometer scale region probed without any indication of phase segregation or Sn precipitation. A typical compositional profile
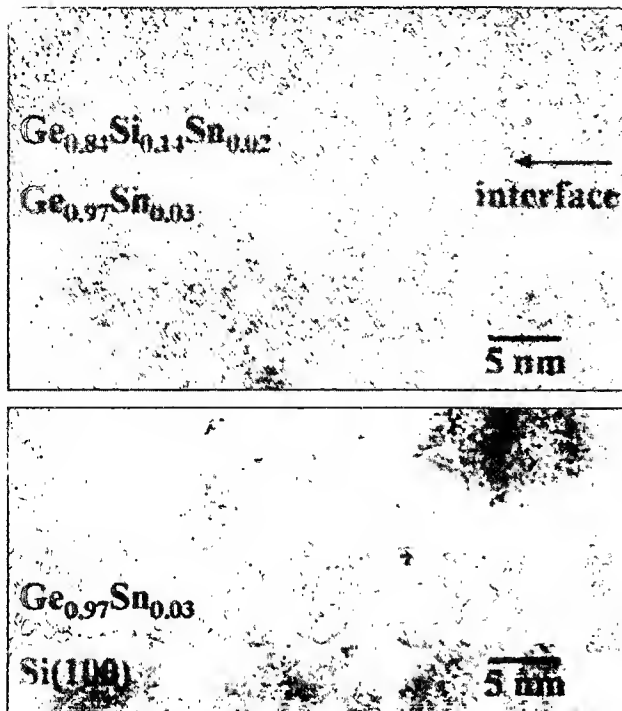
FIG. 3. High-resolution micrographs of $Si_{0.14}Ge_{0.84}Sn_{0.02}$. Top panel shows the $Si_{0.14}Ge_{0.84}Sn_{0.02}/Ge_{0.97}Sn_{0.03}$ interface, demonstrating a virtually defect-free heteroepitaxial character. Bottom panel shows the $Si/Ge_{0.97}Sn_{0.03}$ interface. Edge dislocations are located at the interface and common defects such as stacking faults and twins are visible above the interface.

derived from EDX line scans showing a constant Si distribution across the epilayer is presented in Fig. 4.

The local bonding environment of the Si–Ge–Sn alloys was characterized by Raman spectroscopy. Figure 5 shows the spectrum of a $Si_{0.14}Sn_{0.06}Ge_{0.80}$ sample and is reminiscent of that of Si_xGe_{1-x} alloys, with three main features that are known as the Ge–Ge, Si–Ge and Si–Si peaks. The similarity to Si_xGe_{1-x} shows that the incorporation of Sn does not alter the relative distribution of Si and Ge atoms in the lattice. No
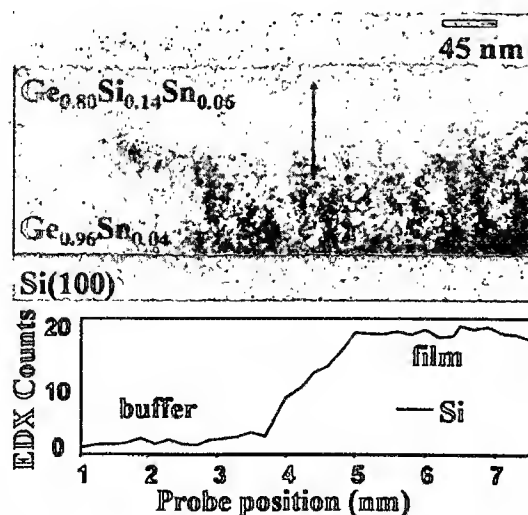

FIG. 4. The top panel is XTEM micrograph of the $Si_{0.14}Ge_{0.80}Sn_{0.06}/Ge_{0.96}Sn_{0.04}/Si$ heterostructure showing the exceptional uniformity of the film thickness. The bottom panel shows an EDX profile of Si across the buffer layer/epilayer interface. The slope at the interface is attributed to Si fluorescence by Ge.
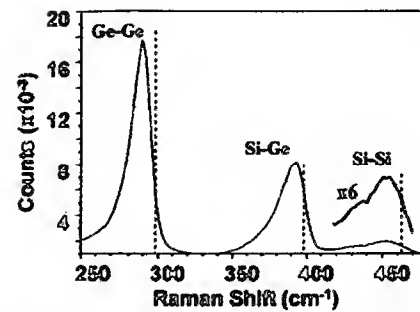

FIG. 5. Raman spectrum of a $Si_{0.14}Ge_{0.80}Sn_{0.06}$ film showing the Si–Si, Si–Ge and Ge–Ge peaks at 454, 393 and 292 cm^{-1}, respectively. The dotted lines represent the expected peak positions for a relaxed film where all the Sn atoms are replaced by Ge atoms.

Sn-related vibrations are obvious in the spectra, presumably due to the low Sn concentration. However, the presence of substitutional Sn is apparent from the measured frequencies of the Raman modes. The dotted lines in Fig. 5 show the expected position[10] of the three main features in $Si_{0.14}Ge_{0.86}$ alloys. Our measured values are clearly downshifted with respect to that shown by the dotted lines, and we can show that this is due to the lattice expansion induced by Sn. Let us consider, for example, the Si–Si mode. In Si_xGe_{1-x} alloys, its frequency is given by $\omega_{Si-Si}=521-68x$.[10] It has been shown that this can be written as[11]

$$\omega_{Si-Si}=521-49x-455 \; \Delta a/a. \tag{1}$$

The second term in Eq. (1) represents the mass disorder and the third term accounts for stretching of the Si–Si bond in Si_xGe_{1-x}. Here Δa is the difference between the lattice constant of the alloy and that of Si. Since Ge atoms have very small displacements for Si–Si modes, we assume that their substitution for even heavier Sn does not have any effect on the first term in Eq. (1). Hence the difference between the measured Si–Si frequency and the corresponding one shown by the dotted line originates entirely from the second term in Eq. (1). If we imagine substituting 6% Ge with 6% Sn, the additional expansion of the lattice is 0.073 Å, which leads to an additional frequency shift of $-7 \; cm^{-1}$. This is in reasonable agreement with the experimental value of $-9 \; cm^{-1}$, particularly in view of the approximations made and the fact that Eq. (1) is most accurate for Si-rich alloys.

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X.   *RELATED PROCEEDINGS APPENDIX*

None.